

Nano-Optics and Nanophotonics

Ole Keller

Quantum Theory of Near-Field Electrodynamics

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With 33 Figures



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To my wife Kaisa and son Sune

Preface

Within the last quarter of a century a new subfield of electrodynamics named *near-field optics* has emerged. In near-field optics, the light–matter interaction on a subwavelength scale is in focus. In the context of the electrodynamics of mesoscopic objects and condensed-matter media of macroscopic size the local-field concept thus is of central importance. Notwithstanding the fact that the overwhelming majority of the experimental studies up to now have dealt with problems in the visible, near-infrared, and near-ultraviolet regions of the electromagnetic spectrum, much of the basic theory covers a broader frequency spectrum. In view of this, I have preferred to use the term *near-field electrodynamics* in the title of the book.

In a sense, all the quantum theory of near-field electrodynamics is contained in the framework of quantum electrodynamics (QED), but, and this is the important point, studies in near-field electrodynamics make it possible for us to see certain aspects of QED in a new perspective. QED is the covering theory of semiclassical electrodynamics in which the electromagnetic field is treated classically and the particle dynamics by quantum mechanics (in its first- or second-quantized form). The semiclassical theory in itself is the covering theory of classical electrodynamics, in which the motion of the individual charged particles is determined by the Newton–Lorentz equation.

It has not been the purpose of this book to cover the many specific theoretical problems in near-field electrodynamics which physicists have been engaged in over the years. Instead, I have sought to give the reader an account of the basic theory, including the theory’s connection to electrodynamics as such. Even with this limited goal a number of important fundamental issues necessarily cannot be covered in a single volume. With the aim of placing the theory of near-field electrodynamics in its proper framework it is unavoidable not to touch upon themes covered in books on general electrodynamics. However, where possible I have attempted to describe such themes with an eye to the near-field perspective. Although many (and perhaps most) of the theoretical studies in near-field electrodynamics have been carried out within the framework of macroscopic (classical) electrodynamics, I have always held the point of view that a proper understanding of field–matter interaction on a subwavelength scale in most cases requires quantum physics. The content of the book reflects this standpoint, and there is no doubt in my mind that the quantum theory of near-field electrodynamics, and in particular its field-quantized version,

will take up a central place in the future. The quantum theory of near-field electrodynamics also influences our view of old subjects and problems, e.g., the spatial localization and confinement theory of transverse photons, a theory which links with the question of diffraction limitation in optics.

In a way, the central topic in near-field electrodynamics is the interplay between radiative and non-radiative (matter-attached) fields. This interplay takes place in a narrow region in the vicinity of matter. I have called this region the rim zone of matter. Theoretical studies of rim-zone electrodynamics appear fascinating and complicated, fascinating because they offer us a fresh view on electrodynamics (optics), and complicated due to the fact that the electromagnetic coupling between objects in rim-zone contact is strong. In the rim zone the irrotational part of the electric field, $\mathbf{E}_L$, is divergence-free, and the criterion $\nabla \cdot \mathbf{E}_L = 0$ I take as a definition of what is meant by “near” in near-field electrodynamics.

We begin the book (Part I) with elements of the microscopic classical theory of electrodynamics, originating in the works of J.C. Maxwell and H.A. Lorentz (and others). In this formulation matter is considered to consist of point-particles. Among other things, the Liénard–Wiechert fields, radiation reaction, multipole electrodynamics, point–dipole interactions, and global and local conservation laws are studied. Electromagnetic Green functions for the electric and magnetic fields play an important role in near-field electrodynamics, and these functions are treated in detail in various representations. Particular emphasis is devoted to the polar and angular spectrum representations. The last representation is of great importance in relation to studies of evanescent electromagnetic fields, and electromagnetic surface and interface waves.

In Part II, we discuss the semiclassical theory of near-field electrodynamics. Here, quantum mechanics is used to describe the particle dynamics, but the electromagnetic field is treated classically. Starting from considerations related to the division into transverse and longitudinal electrodynamics, we go on with a detailed account of the linear nonlocal response theory. This theory forms the basis for local-field calculations in electrodynamics. On the basis of the Liouville equation for the (many-body) density matrix operator the quantum theory of the so-called generalized nonlocal linear response is established. After accounts of the microscopic Ewald–Oseen extinction theorem, my own coupled-antenna theory, transverse and covariant electromagnetic propagators, and principal volume and self-field dynamics, follows chapters devoted to photon wave mechanics (PWM), i.e., the first-quantized theory of the photon. The covariant four-potential formulation of PWM is of particular importance in near-field electrodynamics, because the so-called longitudinal and scalar photons together only affects the physics in the rim zone. Although the covariant covering theory of PWM, namely QED, traditionally has been used in high-energy physics, I advocate the use of the covariant description in near-field electrodynamics, among other things, because it offers us a fresh view on the spatial localization problem for transverse photons emitted from single atoms and mesoscopic objects. It is described why superlocalization in space (spatial confinement to atomic dimension) may occur for the electromagnetic field in the initial moments of its emission from a pure spin transition. A short treatment of

one-particle position operators and spatial localization for massive particles helps one to understand that the lack of perfect spatial localization is shared by the transverse photon and the electron.

Albert Einstein's 1905 analysis of the high-frequency part of Max Planck's black-body radiation law indicated that electromagnetic fields at high frequencies may be considered as consisting of particles (later named photons). With this in mind we discuss the possibilities for establishing an eikonal theory for transverse photons. The limitation on this possibility relates to basic properties in near-field electrodynamics.

In Part III, the relation between QED and near-field electrodynamics is discussed. Due to the importance of Green function and electromagnetic propagator formalisms in rim-zone electrodynamics it is useful to extend the classical Maxwell–Lorentz equations to the operator level. In their quantized form these equations describe the time evolution of the global field–matter system in the Heisenberg picture. The formal form of the equations depends on the choice of gauge. In the Coulomb gauge the set of operator equations becomes form-identical to the classical Maxwell–Lorentz equations, whereas they in the Poincaré gauge take a different form. The Poincaré gauge relates to a specific choice for the generalized polarization and magnetization fields, quantities of substantial importance in the classical description of near-field interactions.

A careful study of field commutator relations, whether it be for free fields or fields in the presence of matter, is a necessity in QED, and the connection of various field commutators to the possibilities for measuring electromagnetic fields in space-time was discussed in detail already in 1933 by Niels Bohr and Leon Rosenfeld. In the wake of the renormalization program developed around 1947 to deal with the problem of infinities in QED, these authors gave a more exhaustive treatment of the question of field and charge measurements in quantum electrodynamics in 1950. In the context of near-field electrodynamics, the commutator between the transverse parts of the vector potential and the electric field turns out to be of particular interest because this commutator in a quite direct manner expresses our inability to localize photons in space beyond the extension of the rim zone. The study of the field commutator relations leads one to integral representations of various covariant scalar propagators, most notably the Jordan–Pauli propagator and the Feynman meson propagator.

The QED description of the nonrelativistic particle–field interaction is studied in some generality and via examples of particular interest in near-field optics and mesoscopic electrodynamics. The link between QED and PWM is established by acting on single-photon wave packet states with certain photon-field operators which relate to the two photon helicity species. The understanding of the photon emission from single atoms (and mesoscopic particles) is of central importance in near-field QED, and we study this emission in some detail for a so-called two-level atom. From the dynamical equations for the coupled two-level atom plus field system a qualitative description of the spontaneous emission process and the Lamb shift can be obtained. Examinations of the particle–particle interaction via exchange of transverse photons lead us to qualitative theories for (1) the delay and magnetic

corrections to the Coulomb interaction between two charged particles, (2) the van der Waals interaction between two electrically neutral particles (or mesoscopic objects), and (3) the Casimir theory for particle–surface interactions.

A study of matter-attached quantized fields is central to near-field QED, and we approach this subject by a manifestly Lorentz-covariant photon description. The covariant quantization of the four-potential raises some fundamental problems, which solution brings us in contact with the Gupta–Bleuler–Lorenz condition and field quantization with an indefinite metric. Subsequently, some efforts are devoted to an introduction of the near-field plus gauge photon concept in QED, and to a discussion of the covariant Feynman photon propagator. Recently, the transverse part of this propagator has turned out to be of importance in connection to studies of field correlations in near-field photon wave mechanics, when this is based on photon position states defined via the transverse part of the vector potential.

Matter-attached fields are unavoidably present in the near-field zone of matter, and in the covariant notation their quantization leads to the scalar and longitudinal photons, and then by a certain unitary transformation to gauge and near-field photons. The conceptual usefulness of the matter-attached field quantization is illustrated by two examples: (1) The interaction between two fixed charges and (2) the radiation of scalar and longitudinal photons from a classical sheet current with negligible quantum fluctuations. Example (1) leads, as it is well-known to a reinterpretation of the Coulomb interaction as being due to an exchange of scalar photons between the two charges. Example (2) obviously is of interest for studies of evanescent fields in QED.

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Part I
Microscopic Classical Theory

Chapter 1

Survey of the Classical Theory

1.1 Why is the Classical Theory Needed?

Notwithstanding that quantum physics is necessary to obtain a good grasp of the theory of near-field electrodynamics classical approaches are still indispensable for several reasons.

Quantum theory is a rational generalization of the classical theory, and the correspondence principle of Niels Bohr [1–4] links the two together. In a certain limit the result obtained by a quantum physical calculation thus agrees with that of a classical calculation. One may illustrate this by an example of importance in mesoscopic optics, viz., the calculation of the linear polarizability of a mesoscopic spherical particle [5]. The quantum calculation aims at a determination of the microscopic nonlocal conductivity of the particle, and may conveniently be carried out on the basis of the equation of motion for the density matrix operator. A knowledge of the conductivity leads directly to a quantum expression for the polarizability. This expression depends on the energies and wave functions of the various stationary states of the mesoscopic particle, as well as on the probability that a given state is occupied. In the Fourier domain of the electromagnetic field, the polarizability depends on the frequency and wave vector of the externally impressed field. As a function of the particle radius (R) the polarizability increases on the average proportional to R^3 , the classical Rayleigh result [6]. Superimposed on this average behavior the polarizability exhibits quantum fluctuations. These fluctuations become less prominent as the radius increases, and the spectrum of the energy eigenstates begins to form a quasi-continuum. Asymptotically, the classical Lorenz–Mie theory for the polarizability of a spherical object is reached [7–9].

For many applications of near-field electrodynamics in the fields of near-field optics and nano-optics it appears sufficient to have an average (effective medium) theory for the physics. In such cases a classical approach is of particular value. In almost all situations a classical calculation is much easier to carry out than a quantum calculation. This, in itself makes the classical approach useful as a starting point for a deeper analysis.

We study the theory of near-field electrodynamics to gain insight in unifying principles, to predict new phenomena, and not least to account for experimental

observations. For the last purpose, it is useful to remember the words of Bohr [10]: “The experimental conditions can be varied in many ways, but the point is that in each case we must be able to communicate to others what we have done and what we have learned, and therefore the functioning of the measuring instruments must be described within the framework of classical physical ideas.” A theoretical account of observations related even to quantum processes (here in near-field electrodynamics) always involve a certain amount of classical theory.

The physics of near-field electrodynamics brings into focus the old question concerning the epistemological difference between classical theory and quantum theory in a fresh and inspiring manner. Alone for this reason it is important to have a clear classical picture of near-field interactions. The central point of quantum theory (and Bohr’s point) can be formulated as follows: No (elementary) phenomenon is a phenomenon until it is a registered (observed) phenomenon [11]. In contrast to this, classical theory tells us that phenomena exists (have a “physical reality” in the words of Einstein, Podolsky, and Rosen [12]) independent of all acts of observation. In both classical and quantum physics isolated systems develop in a deterministic manner in time. All attempts to observe physical properties of an isolated system (object) break its isolation, at least temporarily. The interaction between the system and the measuring apparatus inevitably results in correlations which are conceptually different in classical and quantum physics [13]. In far-field electrodynamic studies these correlations are often (but not always!) so weak that the conceptual difference between classical and quantum measurements can be neglected. In near-field electrodynamics the correlations are in most situations strong, and the joint state of the object and the apparatus appears quite complicated, even in a classical framework. On top of the classical complications, the quantum mechanical measurement process “only” establishes statistical correlations between the states of the object and measuring apparatus [14, 15].

1.2 Classical Electrodynamics: Macroscopic vs. Microscopic Theory

In classical studies of the electrodynamics of macroscopic media, one is often not interested in the detailed behavior of the electromagnetic field over atomic distances. What matters is the average of the field, and the matter properties, over a volume large compared to the volume occupied by a single atom or molecule. Roughly speaking, what is of relevance is an averaging over macroscopically small, but microscopically large, regions. Let us denote such an averaging by $\langle \dots \rangle$. As it is well-known, macroscopic electrodynamics is governed by the following so-called macroscopic Maxwell equations [16–19]:

$$\nabla \times \langle \mathbf{E} \rangle = -\frac{\partial}{\partial t} \langle \mathbf{B} \rangle, \quad (1.1)$$

$$\nabla \cdot \langle \mathbf{D} \rangle = \langle \rho \rangle, \quad (1.2)$$

$$\nabla \times \langle \mathbf{H} \rangle = \langle \mathbf{J} \rangle + \frac{\partial}{\partial t} \langle \mathbf{D} \rangle, \quad (1.3)$$

$$\nabla \cdot \langle \mathbf{B} \rangle = 0. \quad (1.4)$$

As they stand, the macroscopic Maxwell equations are a set of eight equations involving the four fields $\mathbf{E}$, $\mathbf{B}$, $\mathbf{D}$, and $\mathbf{H}$. It is a consequence of (1.2) and (1.3) that the “free” charge ($\langle \rho \rangle$) and current ($\langle \mathbf{J} \rangle$) densities satisfy the equation of continuity, $\nabla \cdot \langle \mathbf{J} \rangle + \partial \langle \rho \rangle / \partial t = 0$. To close the set of equations in (1.1)–(1.4), these are supplemented by so-called constitutive relations connecting the “derived” electric ($\langle \mathbf{D} \rangle$) and magnetic ($\langle \mathbf{H} \rangle$) fields to the “primary” electric ($\langle \mathbf{E} \rangle$) and magnetic ($\langle \mathbf{B} \rangle$) fields [19–22]:

$$\langle \mathbf{D} \rangle = \langle \mathbf{D} \rangle (\langle \mathbf{E} \rangle, \langle \mathbf{B} \rangle), \quad (1.5)$$

$$\langle \mathbf{H} \rangle = \langle \mathbf{H} \rangle (\langle \mathbf{E} \rangle, \langle \mathbf{B} \rangle). \quad (1.6)$$

The constitutive relations describe the electric and magnetic response of the “bound” charges to the primary electromagnetic field, in an average sense. In addition to (1.5) and (1.6), a “generalized Ohm’s law,”

$$\langle \mathbf{J} \rangle = \langle \mathbf{J} \rangle (\langle \mathbf{E} \rangle, \langle \mathbf{B} \rangle), \quad (1.7)$$

is needed to account for the average response of the “free” charges to the field. The constitutive relations in (1.5)–(1.7) in general have a complicated form. Basically, they originate in equations of motions for the charged particles in the selfconsistent (here macroscopic) electromagnetic field.

To obtain the actual (physical) solution of (1.1)–(1.7) also a study of the relevant initial-value problem is needed. In many situations this problem is difficult to solve in a satisfactory manner.

The macroscopic scheme outlined above often is employed even in near-field electrodynamics, where physical phenomena on a subwavelength scale are in focus [23–25]. Great caution must be exercised if the scheme is used in the optical regime, and the results obtained (predicted) in general should be taken with a grain of salt. In nano-optics, where one aims at an understanding of optical phenomena on the nanometer scale, the spatial averaging procedure of macroscopic electrodynamics certainly may be doubtful.

Classical electrodynamics can be based on a quite different scheme in which in a way no spatial averaging procedure is needed. The scheme is based on the so-called microscopic Maxwell–Lorentz equations, which are presented in the following chapter ((2.1)–(2.4)). These equations dates back to Lorentz, who introduced atomic concepts into Maxwell’s theory, in his attempts to “separate ether and matter [26, 27].” In the Lorentz programme only the microscopic $\mathbf{E}$ - and $\mathbf{B}$ -fields appear, and in general these fluctuate rapidly in space over atomic distances. The material particles are considered as charged point-particles, and in the classical Maxwell–Lorentz equations only the current ($\mathbf{J}$) and charge (ρ) densities of these particles appear on the matter side [16–18]. In order to obtain a closed set of equations

for the microscopic classical approach, the Maxwell–Lorentz equations are supplemented by the Newton–Lorentz equations of motion for the various point-particles; see (2.30).

What has been gained in going from macroscopic to microscopic classical electrodynamics? From a quantum mechanical point of view, the correspondence principle leads to the microscopic classical Maxwell–Lorentz theory, an important fact for the quantum theory of near-field electrodynamics. The microscopic electrodynamic field ($\mathbf{E}$, $\mathbf{B}$) concept remains its validity on the atomic length scale (and below). This does not mean that the Maxwell–Lorentz theory can be trusted on the atomic length scale, but if one calculates the microscopic current and charge densities of the particles via the nonrelativistic Schrödinger equation or, if needed, via the Dirac equation, and *not* by means of the Newton–Lorentz equation, a theory valid on the atomic length scale emerges. For most purposes in near-field electrodynamics this so-called microscopic semiclassical theory is a good starting point. The word semiclassical here refers to the fact that the electromagnetic field is treated as a classical (unquantized) quantity. When it comes to classical studies of the near-field interaction between just a few atomic particles the microscopic Maxwell–Lorentz approach is indispensable.

1.3 Maxwell–Lorentz Electrodynamics

Most of the material presented in Part I is based on the framework offered us by the microscopic classical theory of electrodynamics, and the purpose of Chap. 2 is to review and discuss basic aspects of the Maxwell–Lorentz approach with a view to subsequent developments in the quantum theory of near-field electrodynamics.

The potential formulation of the Maxwell–Lorentz theory is emphasized because it is of central importance in near-field electrodynamics. The redundancy in the potentials only affects the rotational-free part of the vector potential and the scalar potential, and the relevant combination of these quantities relates exclusively to the matter-attached part of the electromagnetic field. This part is nonvanishing only in the near-field zone of matter. The gauge freedom allows one a certain flexibility in the description of near-field interactions, a circumstance of great importance in both the semiclassical and field-quantized theory, as we shall realize later on. In the Lorenz gauge, simple and form-identical inhomogeneous wave equations appear for the scalar and vector potentials. The most general and physically acceptable, integral solutions to these equations have the retarded scalar (Huygens) propagator as kernel. With a knowledge of the Lorenz-gauge potentials it is easy to determine the electric and magnetic fields, but one cannot from the standard solutions conclude that these fields are retarded (with the vacuum speed of light) in the near-field zone of matter. From a fundamental point of view the electromagnetic field of a single moving point-charge is of particular interest. From the potentials in the Lorenz gauge, the so-called Liénard–Wiechert potentials, we obtain the electric and magnetic fields of the point-particle. Each of these fields divides naturally into two parts, named

the velocity and acceleration field. Only the velocity field is present if the particle moves with uniform velocity (in the given inertial frame), and this field, also called the attached field, plays an important role in near-field interactions.

Since the dynamical Maxwell–Lorentz and Newton–Lorentz equations exhibit translational invariance in time and space, and rotational invariance in space, the total energy, the total momentum, and the total angular momentum of the global field-particle system are time independent quantities, as we show by a direct calculation. Besides these global conservation laws, one has related local conservation laws of great importance in near-field electrodynamics, not least for conceptual reasons. Perhaps, these laws take the most physical transparent forms when matter, as here, is treated as consisting of an assembly of point-particles [28]. The local energy conservation leads to microscopic expressions for the energy density and energy flow (Poynting vector) of the electromagnetic field. The local momentum conservation allows us to identify the momentum density of the field, and to introduce a stress tensor for the particle-field system. This tensor consists of additive parts from the electromagnetic field (the Maxwell stress tensor (multiplied by -1)) and the point-particles. The local momentum conservation law is important for the studies of, e.g., mechanical forces in near-field optics [29–31] and on atoms [32–34] and mesoscopic (and nano-sized) objects [35]. A classical account for the forces acting on the atoms and molecules in confined fields, and for the radiation pressure (light drag) phenomenon [36], can be made on the basis of the local momentum conservation law. The angular momentum light drag effect [37–39] can be studied starting from the local conservation law for the angular momentum, possibly extended to the semiclassical level in the case of mesoscopic objects [40–42].

1.4 The Standard Green Functions (Not Propagators)

In the Lorenz gauge the four-vector potential is related to the four-current density by means of an integral relation where the kernel is the Huygens propagator. This propagator describes how light spreads out from a source point in space-time. Since the Huygens propagator is nonvanishing (and in fact singular) only on the light cone the interpretation at first sight perhaps appears satisfactory from the point of view of special relativity. However, one must not forget that the four-potential is not an observable quantity in physics. With this in mind, it seems of interest to establish a propagator formalism which relates the electric and magnetic fields to the three-current density. Within the so-called scalar theory of scattering (diffraction) the Huygens propagator continues to be the relevant kernel for the description, but the scalar approach is an approximation [43, 44].

In near-field electrodynamics it has for many years been popular to base theoretical studies on what I here call the *standard Green function* formalism [18, 24, 45–48]. In Chap. 3, the standard Green functions (now dyadic quantities) relating respectively the electric field and magnetic field to the current density of the Maxwell–Lorentz theory are determined and discussed. As everyone else, we carry out the

calculations in the space-frequency domain, *but*, and this is an important point, *we do not say that the result can be taken back to the space-time domain by Fourier transformation, if wished*. From the perspective of near-field electrodynamics we face what might seem to be a conceptual problem: The near-field part of the standard Green function which relates the electric field to the current density does not exist in the space-time domain. This fact is the reason that I use the term standard Green function and not the name standard propagator, as many people do. The root of the above-mentioned problem is the fact that it is the photon field which propagates (with the vacuum speed of light), and this field is associated only to the divergence-free (transverse) part of the electromagnetic field. The related so-called transverse propagator has been studied in [5, 49–51]. The total electric field has a rotational-free part in the near-zone of matter, and if this part is subtracted we arrive at a genuine propagator relation between the transverse electric field and the current density, as we shall realize in Chap. 14. In a quantum context, where the matter field is a continuum field in the probabilistic sense, a related problem arises for the standard Green function for the electric field if the “point of observation” is inside matter: The spatial integral of the Green function is only conditionally convergent, a physically unacceptable feature. The solution of this aspect of the problem is also given in Chap. 14 (see also [45]).

1.5 Evanescent Electromagnetic Fields

The information contained in the standard Green functions $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_M(\mathbf{R}; \omega)$, which relate the electric and magnetic fields to the particle current density, can be represented in a variety of different forms, which basically are physically equivalent. All the forms have in common that they belong to the microscopic Maxwell–Lorentz equations in the frequency (ω) domain. They differ in the manner in which the spatial ($\mathbf{R}$) information is represented. For investigations of a given problem one form of representation can be more useful than the others. In studies of the electrodynamics of atomic, molecular, and mesoscopic objects which linear extensions are (much) less than the relevant wavelengths of the electromagnetic field the standard Green functions are most often given in spherical coordinates. In these coordinates the local unit vectors and the magnitude $R = |\mathbf{R}|$ appear in the Green functions. The R -dependence contains terms proportional to R^{-1} , R^{-2} , and R^{-3} . A term proportional to R^{-3} only appears in the Green function relating to the electric field, and it is this part we referred to as the near-field part of $\mathbf{G}(\mathbf{R}; \omega)$ in the previous section.

If one, at least as an attempt, seeks to make a spatial Fourier transform of the standard Green functions one arrives at a plane-wave (wave vector $\mathbf{q}$) representation of these ($\mathbf{G}(\mathbf{q}, \omega)$, $\mathbf{G}_M(\mathbf{q}, \omega)$). The assumption of the existence of Fourier integral transformations turns out to be incorrect, since $\mathbf{G}(\mathbf{q}, \omega)$ and $\mathbf{G}_M(\mathbf{q}, \omega)$ have poles. Nevertheless, closely related integral representations do exist for $\mathbf{G}(\mathbf{R}; \omega)$ (see also [50]) and $\mathbf{G}_M(\mathbf{R}; \omega)$, and as we shall see later on in this book, these representations are extremely useful. In Chap. 4, we use the plane-wave representation

as a springboard for the introduction of the so-called mixed representation of the standard Green functions. In this representation, also called the angular spectrum representation [44, 52, 53], a Fourier expansion is made in only two coordinates, say X and Y , leading to $\mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega)$ and $\mathbf{G}_M(Z; \mathbf{q}_{\parallel}, \omega)$, where $\mathbf{q}_{\parallel}$ is the wave vector in the XY -plane. The two-dimensional plane-wave expansion is useful in (near-field) studies of the electrodynamics of plane structures (surfaces, interfaces, sheets and layered media), and to a certain extent for the description of the electrodynamic interaction between mesoscopic (or microscopic) particles and plane structures.

The theoretical studies of the electromagnetic coupling between a small particle and a planar surface have a 100-year-old history, starting around 1909 with Sommerfeld's theory for the radiation from an electric dipole oriented vertically above a conducting medium (ground) [54]. In Sommerfeld's asymptotic solution electromagnetic surface waves, investigated earlier by Zenneck [55], appear. A few years later, in 1911, Hörschelmann analyzed the radiation from a horizontally oriented dipole [56]; see also [57]. In Sommerfeld's and Hörschelmann's calculations an expansion of the field in cylindrical coordinates was used. In an important paper, dealing with the propagation of electromagnetic waves over a conducting sphere, Weyl derived a new contour integral representation of a diverging spherical scalar wave [58]. In this representation the mode functions are so-called inhomogeneous waves (more on these below). For a particular contour the Weyl representation provides us with a decomposition of the spherical wave into homogeneous and evanescent field modes, the angular spectrum representation. The early developments in the field is summarized in [59]. Almost two decades ago the Weyl expansion was employed by Agarwal in a theoretical study of the optics of an atom placed in front of a phaseconjugating mirror [60]. Further analyses were made by Hendriks and Nienhuis [61], Milonni et al. [62], Arnoldus and George [63], Agarwal and Gupta [64]. The work of Agarwal inspired me to suggest that phaseconjugation of the field from the tip of a near-field microscope would allow one to focus light beyond the classical diffraction limit [65], an idea which was confirmed experimentally shortly afterwards [66]. An account of the microscopic theory for phaseconjugation from a mesoscopic particle is given in [67]; see also [40], Part B. The question of phaseconjugation of evanescent waves plays an important role for the studies in [60–67], and for further analyses of this the reader is referred to [68, 69], and references therein. Because the field from a point-charge has a singularity at the position of the charge, a rigorous derivation of the Weyl representation of a spherical wave requires some care [70]. The dipole–surface interaction gives rise to a mutual attraction, also found between a pair of parallel, uncharged, conducting plates in vacuum. The attraction, referred to as the Van der Waals attraction, was calculated originally by Casimir [71] in 1949; see also Casimir and Polder [72]. From a quantum electrodynamic point of view, the attraction can be accounted for by assuming that the related force is a consequence of the separation-dependent energy in the vacuum field trapped between the plates [73, 74]. The Weyl expansion has been used by Agarwal in a study of basic aspects of quantum electrodynamics in the presence of dielectrics and conductors [75]. Theoretical studies of the electrodynamic interaction between an electric dipole and a planar (metallic) medium

exhibiting a so-called nonlocal (spatially dispersive) response have also been carried out in the nonretarded regime [76], and with retardation effects included [77, 78], and the results obtained used in calculations of the surface-dressed dipole polarizability. The renormalized polarizability agrees with that obtained in a local approach [79, 80]. The dipole emission near planar interfaces is also discussed in the book by Novotny and Hecht [24], and here further references of interest in nano-optics are listed.

Under certain conditions an evanescent field may be generated by a current sheet, as we shall see. In a sense sheet electrodynamics shows the evanescent field concept in its simplest form, and starting from the result for a single sheet the evanescent fields belonging to more complicated layered structures can be determined by superposition. Evanescent fields play a key role in studies of surface electromagnetic waves; see [24, 25, 81–88], and references therein. In the condensed matter physics literature these waves are commonly referred to as surface polaritons. Roughly speaking a surface polariton is an admixture of the electromagnetic field and a collective particle excitation that propagates along the surface of a medium, or along the interface between two media. The strength of the electromagnetic field associated with a surface polariton decays exponentially as one moves away from the interface into either medium. Surface electromagnetic waves are of particular importance when carried by (bound to) a metal surface, and in the literature they are called surface plasmaritons, surface plasmon polaritons, or just surface plasmons. In the context of near-field optics and nano-optics the study of optical phenomena related to surface waves on metals recently has been termed plasmonics or nanoplasmonics [24]. The overwhelming majority of the theoretical (numerical) calculations describes the metal response on the basis of macroscopic (local) electrodynamics. The diversity of electromagnetic surface phenomena, which one catches a glimpse of when microscopic (nonlocal) response theory is used [84, 89–95] has not been very well explored theoretically nor experimentally up to now. To understand the basic physical properties of surface polaritons bound to the surface of a (BCS) superconductor [96–98] microscopic electrodynamics is necessary [99–102]. Surface electromagnetic waves can be generated (excited) by various methods. Thus, the substantial increase in the interest of surface polaritons which appeared around 1970, mainly was due to excitation schemes suggested by Otto [103] and Kretschmann [104]. In the wake of the birth of near-field optics the use of local (dipole-like) excitation (and detection) methods for surface modes gained renewed interest in the scientific community, and the tremendous recent interest in studies of surface polaritons is bound up with the scanning near-field optical microscopy technique [24, 25]. Evanescent fields also show up when a plane monochromatic electromagnetic wave is incident on a planar dielectric (glass)-vacuum interface at an angle larger than the critical angle. On the vacuum side the electromagnetic field decays exponentially with the distance from the interface. Although the energy density of the evanescent field is nonzero, no energy is transported away from the interface. Frustrated total internal reflection (FTIR) results if a second planar dielectric is brought within an optical wavelength from the first. From a fundamental point of view FTIR is the paradigm of optical tunneling [105–107], and it has been

maintained that photon tunneling is a near-field phenomenon which originates in our inability to localize a photon completely in space [108, 109]. There are certain indications that information on the photon tunneling phenomenon may be obtained from studies of the Goos–Hänchen shift [110–113], a phenomenon which shows up in FTIR experiments. A mixed representation also can be used to describe the current density of a moving point-charge. If the particle trajectory is confined to lie in a plane, a classical expression for the related sheet current density can be established. In near-field electrodynamics it is of importance to investigate also the (cycle-averaged) field momentum density outside the current sheet. We do this paying particular attention to the case of evanescent modes.

Starting from the two-dimensional plane-wave expansion other useful representations of the Huygens propagator and the standard Green functions can be obtained. Thus, for studies of the electrodynamic interaction between a small particle (possibly atom or molecule) and a planar structure it may be advantageous to describe the interaction over the $\mathbf{q}_{\parallel}$ -plane in polar coordinates [50, 114]. The angular integrations associated with the magnetic part of the standard Green function thus can be expressed in terms of Bessel functions of the first kind and zero and first order, for instance. For the electric part of the Green function also the Bessel function of the first kind and second order appears. Altogether, one ends up with a representation of the various Green functions in which only a single integral over the magnitude of $\mathbf{q}_{\parallel}$ ($0 \leq q_{\parallel} < \infty$) enters. The region $0 \leq q_{\parallel} \leq \omega/c_0$ (c_0 is the vacuum speed of light) is associated with homogeneous waves, and the region $\omega/c_0 < q_{\parallel} < \infty$ is connected to evanescent modes. If a different set of variables is used for the integration over the $\mathbf{q}_{\parallel}$ -plane, one may express the Green functions as a contour integral in a complex α -plane. A segment along the $\Re\alpha$ -axis now gives the homogeneous wave contribution, and a segment parallel to the $\Im\alpha$ -axis associates to the evanescent modes. By modifying the contour above one can obtain an expansion of the Green functions in terms of so-called generalized inhomogeneous waves [53, 58, 70]. For these waves the surfaces of constant amplitude and of constant phase are distinct, except for special values of the variables.

1.6 Multipole Electrodynamics: A Richly Faceted Subject

The theoretical analysis of field–matter interactions is simplified in cases where the linear extension of the particle system (object) is much smaller than the “relevant” wavelengths of the electromagnetic field. What we mean by the word relevant depends on the context. In order to exemplify this let us consider the interaction of a monochromatic external (incoming) field with an object of extension much less than the wavelength of the external field. During the interaction local fields of different wavelengths are generated inside the object and these fields do not have wavelengths which are large in comparison with the linear size of the object. Despite this, the relevant wavelength is that of the externally impressed field in this case. If the monochromatic external field is replaced by a quasi-monochromatic field of the

same mean frequency, the relevant wavelengths are those of this field. From the point of view of electrodynamics the object may be characterized as mesoscopic. An object which appears mesoscopic when subjected to an external field may also be characterized as mesoscopic in a field emission process if the dominating wavelengths of the radiated field all are much larger than the electronic size of the object. The field–matter interaction in the case of mesoscopic objects often is characterized as mesoscopic electrodynamics. Nano-optics, which deals with the electromagnetic interaction between visible (or infrared or ultraviolet) light and nano-sized objects, is a form of mesoscopic electrodynamics. The optical near-field interaction with material structures may also be characterized as a sort of mesoscopic electrodynamics.

The prevailing microscopic classical current density, $\mathbf{J}(\mathbf{r}, t)$, in a mesoscopic object can often with advantage be described in terms of a so-called moment expansion, in which only terms of the lowest orders are retained. The spatial integral (zeroth-order moment) of $\mathbf{J}(\mathbf{r}, t)$ over the mesoscopic object gives the so-called electric dipole current density, $\mathbf{J}^{\text{ED}}$, of the object (at a given time). The spatial first-order moment of $\mathbf{J}(\mathbf{r}, t)$, a tensorial quantity, gives the sum of the electric quadrupole ($\mathbf{J}^{\text{EQ}}$) and the magnetic dipole ($\mathbf{J}^{\text{MD}}$) moments of the current density distribution. The symmetric part of the tensor is the EQ-moment, and the anti-symmetric part is the MD-moment. The moments $\mathbf{J}^{\text{ED}}$ and $\mathbf{J}^{\text{EQ}}$ are just the time derivatives of the well-known electric dipole ($\mathbf{p}(t)$) and quadrupole ($\mathbf{Q}(t)$) moments of a point-charge distribution. The quantity $\mathbf{J}^{\text{MD}}$ relates in a simple fashion to the magnetic dipole moment ($\mathbf{m}(t)$) of a point-charge distribution, a moment which in turn can be expressed in terms of the (relativistic) orbital angular momenta of the individual point-particles.

In the space-frequency domain the electric ($\mathbf{E}^{\text{ED}}(\mathbf{r}; \omega)$) and magnetic ($\mathbf{B}^{\text{ED}}(\mathbf{r}; \omega)$) fields generated by $\mathbf{p}(\omega)$ can be expressed in compact form with the help of the standard Green functions $\mathbf{G}(\mathbf{r}; \omega)$ and $\mathbf{G}_M(\mathbf{r}; \omega)$, respectively. The fields $\mathbf{E}^{\text{MD}}$ and $\mathbf{B}^{\text{MD}}$ generated by $\mathbf{m}(\omega)$ can also be expressed in terms of the standard Green functions. In this case $\mathbf{G}_M(\mathbf{r}; \omega)$ relates to $\mathbf{E}^{\text{MD}}(\mathbf{r}; \omega)$, and $\mathbf{G}(\mathbf{r}; \omega)$ to $\mathbf{B}^{\text{MD}}(\mathbf{r}; \omega)$. As the reader may have anticipated, the fields $\mathbf{E}^{\text{EQ}}(\mathbf{r}; \omega)$ and $\mathbf{B}^{\text{EQ}}(\mathbf{r}; \omega)$ which are generated by $\mathbf{Q}(\omega)$ relate to the third rank tensors $\nabla \mathbf{G}(\mathbf{r}; \omega)$ and $\nabla \mathbf{G}_M(\mathbf{r}; \omega)$.

In near-field electrodynamics one is faced with a complicated interplay between the divergence-free (transverse) and rotational-free (longitudinal) parts of the electromagnetic field. This interplay is important for our understanding of the space-time generation and destruction of photons in their interaction with matter, whether it be in the context of the first or second-quantized theory, and for fundamental studies of our ability to localize photons in space-time. In mesoscopic electrodynamics it is therefore fruitful to seek to establish a multipole formalism which respects the division of the electromagnetic field into its transverse and longitudinal parts [19, 115–117]. In Sects. 5.4 and 5.5, a systematic approach for higher-order multipoles is developed for the transverse part of the field. The calculations are carried out in the space-frequency domain, and we start by considering the electromagnetic field in a source-free region of space. In such a region the electric ($\mathbf{E}(\mathbf{r}; \omega)$) and magnetic ($\mathbf{B}(\mathbf{r}; \omega)$) fields satisfy the Helmholtz equation, and so

do the scalar quantities $\mathbf{r} \cdot \mathbf{E}(\mathbf{r}; \omega)$ and $\mathbf{r} \cdot \mathbf{B}(\mathbf{r}; \omega)$ because the $\mathbf{E}$ - and $\mathbf{B}$ -fields are divergence-free in vacuum. In preparation for the introduction of the so-called transverse electromagnetic multipole waves one seeks the general solution to the Helmholtz equation for the scalars $\mathbf{r} \cdot \mathbf{E}$ and $\mathbf{r} \cdot \mathbf{B}$ in spherical coordinates. The solution can be written as a double sum with parameters J and M . The parameter J can take on the values $J = 0, 1, 2, \dots$, and for a given value of J the possible M 's are $M = -J, -J + 1, \dots, 0, \dots, J - 1, J$. Not surprisingly, these parameters are identical to those entering the quantum theory for the orbital angular momentum. Each (J, M) -term consists of a product of a spherical harmonic (Y_{JM}) and a radial function. With an eye to studies of radiation problems, the radial function is given in the form of a superposition of spherical Hankel functions of the first ($h_J^{(1)}$) and second ($h_J^{(2)}$) kind and order J . The electromagnetic multipole waves are divided into two groups: (1) Electric multipole waves (superscript (E)) for which $\mathbf{r} \cdot \mathbf{B}_{JM}^{(E)} = 0$, and (2) magnetic multipole waves (superscript (M)) for which $\mathbf{r} \cdot \mathbf{E}_{JM}^{(M)} = 0$. The subscript JM indicates that there belongs a multipole wave to each combination of J and M . In the transverse-electromagnetic-multipole-wave decomposition of the general solution to the free-space Maxwell equations still appears linear combinations of the Hankel functions $h_J^{(1)}$ and $h_J^{(2)}$, but instead of the spherical harmonics Y_{JM} we now find the so-called vector spherical harmonics $\mathbf{X}_{JM} \propto i^{-1} \mathbf{r} \times \nabla Y_{JM}$.

In the multipole wave expansion of the electromagnetic field in source-free regions of space appears yet arbitrary so-called electric and magnetic multipole coefficients, which basically give the strengths of the various multipole fields. In order to determine these coefficients one needs to know the current density distribution ($\mathbf{J}(\mathbf{r}; \omega)$) in the source which generates the field.

The examination of the connection between the multipole field strengths and the source current density distribution gives us a glimpse of the important question of how to choose appropriate field variables in the source domain. A key point here is to work with a new “electric-field” variable which is divergence-free everywhere in space (the magnetic field *is* transverse everywhere according to the Maxwell theory). The new electric-field variable ($\mathcal{E}$) is given by $\mathcal{E}(\mathbf{r}; \omega) = \mathbf{E}(\mathbf{r}; \omega) + i \mathbf{J}(\mathbf{r}; \omega) / (\epsilon_0 \omega)$. In Sect. 10.4 we shall introduce the generalized electric displacement field $\mathbf{D}$ and the generalized magnetization $\mathbf{M}$ [118, 119]. In terms of these, one has

$$\epsilon_0 \mathcal{E}(\mathbf{r}; \omega) = \mathbf{D}(\mathbf{r}; \omega) + \frac{i}{\omega} \nabla \times \mathbf{M}(\mathbf{r}; \omega), \quad (1.8)$$

as the reader may show after having studied Sect. 10.4. The $\mathbf{D}$ -field plays an important role in linear nonlocal response theory, and for studies of near-field aspects of the photon emission from micro- and mesoscopic sources. It is possible to make the choice $\mathbf{M} = \mathbf{0}$ without changing any physical properties of the field-particle system as we shall learn in Sect. 10.4.1. With such a choice the new transverse field variable $\mathcal{E}$ is just the generalized displacement field (divided by ϵ_0). Via the Helmholtz equations for $\mathbf{r} \cdot \mathcal{E}$ and $\mathbf{r} \cdot \mathbf{B}$, one is able to express the actual electric and magnetic multipole coefficients in terms of space-integrals involving $\nabla \times \mathbf{J}$ and $\mathbf{J}$, respectively.

As we shall see, the multipole expansion of the source current density distribution is useful in studies of the rate of energy, momentum, and angular momentum transfer to a mesoscopic particle from a prescribed external field.

1.7 Local Electromagnetic Fields and Resonances

In near-field electrodynamics the local field concept is of central importance. Thus, if one has a knowledge of this field *all* electrodynamic properties of the medium under study can be predicted. Although quantum physics is needed for a rigorous calculation of local fields, because these vary on a length scale (much) shorter than that of the externally impressed field in most cases, it is of some interest to study local fields in the framework of the microscopic Maxwell–Lorentz equations. For an assembly of point-particles the local electric field at a given point ($\mathbf{r}$) in space is the sum of the external field at this point and the fields generated at $\mathbf{r}$ by the various particles of the system [5, 24, 25, 114, 120–129]. The field generated by a given point-particle is not known a priori, however, because the current density distribution of this particle, which is the source of the emitted field, is determined by the local field acting on the particle. To cut the Gordian knot, one must in a selfconsistent manner determine the local fields acting on all the particles in the system. This task is a formidable difficult one in general. If we treat the particles as electric dipoles, and limit ourselves to linear response theory, the task can be solved. A supermatrix $(\mathcal{U} - \mathcal{T})^{-1}$ relates the local fields at the sites of the, say N , dipoles to the external fields at these sites. The quantity $\mathcal{T}$ contains the electric-dipole polarizabilities of the various particles, and the Green functions $\mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega)$ [$(i, j) = 1, 2, \dots, N$] describing the field communication between all pairs, (i, j) , of dipoles. In some cases the particles are so close to each other that only the near-field part of the $\mathbf{G}$'s needs to be retained. Once the selfconsistent solution for the electric field on the dipole sites has been obtained the local field easily can be determined everywhere else in space. The procedure described above incorporates all kinds of multipole scattering between the electric dipoles, and from the general result the Born series approach to the N -particle scattering problem can be established by making a power series expansion of $(\mathcal{U} - \mathcal{T})^{-1}$ in $\mathcal{T}$.

In a closed system no external fields act, and possible selfconsistent solutions for the local field therefore are selfsustaining. For an assembly of electric dipoles self-sustaining solutions must satisfy the condition $\text{Det}\{\mathcal{U} - \mathcal{T}\} = 0$, where Det stands for determinant. The inevitable presence of irreversible electronic damping mechanisms and spontaneous emission makes all systems open to some extent, perhaps with the exception that the whole universe may be considered closed. Selfsustaining solutions are also called local-field resonances, and this name is also used to cover the resonances one may obtain in weakly open systems. Roughly speaking, a local-field resonance occurs whenever a component of the supermatrix $(\mathcal{U} - \mathcal{T})^{-1}$ has a deep minimum. Local-field resonances can occur at certain frequencies $\omega = \omega_{\text{Res}}$, or at a given frequency for certain spatial arrangements of the dipole positions.

In the last case, which most often occurs in few-particle systems, one speaks of a configurational resonance.

The classical multipole scattering among magnetic dipole, and between electric quadrupoles, can of course be studied by analogy with the treatment for electric dipoles.

1.8 Radiation Reaction in a Classical Perspective

In the procedure for classical local-field calculations, which we briefly described in the foregoing section, the radiative reaction which the field emitted from a point-particle exerts on the particle itself was not taken into account. The radiation reaction problem raises deep questions in electrodynamics, and the problem cannot be dealt with in a satisfactory manner in the framework of classical electrodynamics. Nevertheless, it certainly is worthwhile to study the phenomena in a purely classical context because this gives us some insight in the problems we are facing [19, 130–133]. Nonrelativistic and fully relativistic quantum mechanical treatments have been given by Moniz and Sharp [134], and by Low [135], respectively.

An electrically charged point-particle emits energy when accelerated, and the radiative energy loss affects the motion of the particle. In classical electrodynamics a point-charge placed in a prescribed (external) electromagnetic field moves according to the Newton–Lorentz equation. To account for the radiative energy loss some force, called the radiation reaction force, must act on the particle besides the force exerted by the external field. In the nonrelativistic Abraham–Lorentz approach the radiation reaction force is determined in some approximate and time-averaged sense via the instantaneous power radiated by the particle’s acceleration field [19, 130, 136–138]. By demanding that the negative of the work carried out on the particle by the yet unknown radiative reaction force in a *certain* time interval equals the power radiated in this interval one finds that the radiative reaction force is proportional to the time derivative of the particle’s instantaneous (!) acceleration. To reach this conclusion the particle motion must have such a form that the scalar product of the particle velocity and acceleration has the same value at the two endpoints of this “certain” time interval.

From our nonrelativistic classical standpoint the radiation reaction effect is of importance if the relative change in the particle acceleration is appreciable on a time scale $\tau_0 = Q^2/(6\pi\epsilon_0 mc_0^3)$, where Q and m are the charge and mass of the particle. For the electron $\tau_0 \approx 6.3 \cdot 10^{-24}$ s. Among other doubtful consequences, the Abraham–Lorentz model predicts a preacceleration effect on a time scale of the order of τ_0 [116, 130]. To observe such an effect the external force must be switched on over a time interval $\sim \tau_0$, an impossibility for classical interactions. The classical theory for the radiation reaction is useful in physical optics, where it gives an important contribution to the electric dipole polarizability, for instance [18]. As a part of the particle’s “inner” dynamics the so-called (radiation reaction) dressed polarizability is the observable quantity in (near-field) electrodynamics. The electric radiation

reaction field $\mathbf{E}_{\text{RR}}(\omega)$ of an electric dipole (moment $\mathbf{p}(\omega)$) also can be obtained via the standard Green function $\mathbf{G}(\mathbf{R}; \omega)$ if one near $\mathbf{R} = \mathbf{0}$ keeps the small imaginary part of $\mathbf{G}$. Because this part varies only little on a length scale comparable to the linear extension of a mesoscopic object, the radiative reaction on such an object does not depend (significantly) on the electronic structure of the object. Via the Green function $\mathbf{G}_{\text{M}}(\mathbf{R}; \omega)$ the magnetic radiation reaction field $\mathbf{B}_{\text{RR}}(\omega)$ on a magnetic dipole (moment $\mathbf{m}(\omega)$) is easily calculated. The duality between the electric and magnetic fields shows that $|\mathbf{E}_{\text{RR}}(\omega)|/|\mathbf{p}(\omega)| = c_0^2 |\mathbf{B}_{\text{RR}}(\omega)|/|\mathbf{m}(\omega)|$.

In the classical relativistic domain the modification of a charged point-particle's motion by radiation reaction is described by the Lorentz–Dirac equation [139–144]. Starting from the derivation of a manifestly covariant expression for the energy-momentum radiation rate, and the conclusion following from the fact an elementary particle keeps its rest mass intact during the radiation reaction process, we end up with the Lorentz–Dirac equation. In order to cancel the rest-mass changing radiation, one suspects that the attached self-field of the particle will be temporarily distorted during the acceleration process. An unaccelerated charged object carries along its velocity field, and in the particle's rest frame this is just the electrostatic Coulomb field. The related field energy is equivalent to some so-called electromagnetic mass in a relativistic context. Observed in an inertial frame moving with respect to the rest frame, the velocity field contributes a self-momentum to the uniformly moving particle. A distortion of the self-momentum appears during accelerated particle motion. In an external (ext) electromagnetic field the transverse vector potential $A_{\text{T}}^{\text{ext}}$ adds a momentum $QA_{\text{T}}^{\text{ext}}$ to the particle, and this momentum spreads over the Coulomb self-field region. As soon as the external magnetic field overlaps this region the attached field momentum starts to be distorted. For an elementary discussion of this aspect the reader is referred to [116].

Chapter 2

Maxwell–Lorentz Electrodynamics in Space-Time

2.1 The Maxwell–Lorentz Equations

The starting point for the microscopic classical theory of the interaction between electrically charged particles is the Maxwell–Lorentz equations [16–19, 145, 146], which relate the electric field $\mathbf{E}(\mathbf{r}, t)$ and the magnetic field $\mathbf{B}(\mathbf{r}, t)$ to the charge density $\rho(\mathbf{r}, t)$ and current density $\mathbf{J}(\mathbf{r}, t)$ as follows:

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t), \quad (2.1)$$

$$\nabla \cdot \mathbf{E}(\mathbf{r}, t) = \frac{1}{\epsilon_0} \rho(\mathbf{r}, t), \quad (2.2)$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \mu_0 \mathbf{J}(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{E}(\mathbf{r}, t), \quad (2.3)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0, \quad (2.4)$$

where ϵ_0 and μ_0 are the vacuum permittivity and permeability, respectively, and $c_0 = (\epsilon_0 \mu_0)^{-1/2}$ is the speed of light in vacuo. The equations above describe the field–matter coupling in space($\mathbf{r}$)-time(t). In the Maxwell–Lorentz equations the electrodynamic properties of matter are described exclusively in terms of $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$, and these quantities relate to the charge and current density of all the microscopic particles. Local conservation of electric charge implies that $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ are not independent, but related via an equation of continuity, which is implicitly hidden in (2.2) and (2.3); see Sect. 2.7.1.

2.2 Vector and Scalar Potentials: Gauge Invariance

The Maxwell–Lorentz equation in (2.4) suggests that the magnetic field is written in the form

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t), \quad (2.5)$$

since the divergence of a curl of a vector is zero. The vector field $\mathbf{A}(\mathbf{r}, t)$ is called the vector potential, and if (2.5) is inserted into (2.1) it appears that

$$\nabla \times \left(\mathbf{E}(\mathbf{r}, t) + \frac{\partial}{\partial t} \mathbf{A}(\mathbf{r}, t) \right) = \mathbf{0}. \quad (2.6)$$

The vector sum in the parenthesis therefore can be written as (minus) the gradient of a scalar quantity $\phi(\mathbf{r}, t)$ called the scalar potential, and hence we get

$$\mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{A}(\mathbf{r}, t) - \nabla \phi(\mathbf{r}, t). \quad (2.7)$$

Ipsa Facto that the electric and magnetic fields are given by (2.5) and (2.7) we have automatically satisfied the two Maxwell–Lorentz equations in which neither $\rho(\mathbf{r}, t)$ nor $\mathbf{J}(\mathbf{r}, t)$ appear; ((2.1) and (2.4)). By insertion of (2.5) and (2.7) into the remaining Maxwell–Lorentz equations ((2.2) and (2.3)) one obtains the following coupled second-order partial differential equations for $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$:

$$\nabla^2 \phi(\mathbf{r}, t) + \frac{\partial}{\partial t} \nabla \cdot \mathbf{A}(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \rho(\mathbf{r}, t), \quad (2.8)$$

$$\square \mathbf{A}(\mathbf{r}, t) - \nabla \left(\nabla \cdot \mathbf{A}(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \phi(\mathbf{r}, t) \right) = -\mu_0 \mathbf{J}(\mathbf{r}, t), \quad (2.9)$$

where

$$\square = \nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \quad (2.10)$$

is the d'Alembertian operator, and $\nabla^2 = \nabla \cdot \nabla (= \Delta)$. In deriving (2.9) we have used the vector relation $\nabla \times (\nabla \times \mathbf{A}) = \nabla \nabla \cdot \mathbf{A} - \nabla^2 \mathbf{A}$. The introduction of the scalar and vector potential simplifies (via a certain gauge choice; see below) the calculation of the electric and magnetic fields generated by prescribed charge and current density distributions, as we shall realize in Sect. 2.3. For the semiclassical (Part II) and field-quantized (Part III) descriptions of (near-field) electrodynamics the potential formulation of the Maxwell–Lorentz equations is indispensable.

There is a certain redundancy in the potentials since the electric and magnetic fields are invariant under the following transformation:

$$\mathbf{A}(\mathbf{r}, t) \rightarrow \mathbf{A}'(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) + \nabla \chi(\mathbf{r}, t), \quad (2.11)$$

$$\phi(\mathbf{r}, t) \rightarrow \phi'(\mathbf{r}, t) = \phi(\mathbf{r}, t) - \frac{\partial}{\partial t} \chi(\mathbf{r}, t), \quad (2.12)$$

where $\chi(\mathbf{r}, t)$ is an arbitrary (yet space- and time-differentiable) function of $\mathbf{r}$ and t . We shall have much more to say about the role of gauge transformations when discussing the quantum theory of near-field electrodynamics.

2.3 The Implicit Solution of the Maxwell–Lorentz Equations

It appears from (2.11) that $\nabla \cdot \mathbf{A}' = \nabla \cdot \mathbf{A} + \nabla^2 \chi$. This freedom to choose arbitrarily the divergence of $\mathbf{A}$ enables one to decouple the differential equations for $\mathbf{A}$ and ϕ in (2.8) and (2.9). With the choice

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial \phi(\mathbf{r}, t)}{\partial t} = 0, \quad (2.13)$$

the equations for $\mathbf{A}$ and ϕ not only separate, they also take the same form, viz.,

$$\square \mathbf{A}(\mathbf{r}, t) = -\mu_0 \mathbf{J}(\mathbf{r}, t), \quad (2.14)$$

and

$$\square \phi(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \rho(\mathbf{r}, t). \quad (2.15)$$

The gauge condition (choice) in (2.13) is called the Lorenz gauge condition, named after Lorenz [147–149]. The reader may be surprised to find that the relation in (2.13) is associated with the Danish physicist Ludvig V. Lorenz, and not the Dutch physicist Hendrik A. Lorentz. Yet, it is a fact that Lorenz in 1867 came to this relation when exploiting the retarded solutions for the potentials [150–152]. The set of equations in (2.13)–(2.15) constitute the framework of Lorenz' electrodynamical theory [19, 147, 148, 153], and the set is equivalent to the microscopic Maxwell–Lorentz equations, written essentially in the covariant form! The Lorenz condition in (2.13) does not fix the potentials completely. Restricted gauge transformations for which the gauge function χ satisfies $\square \chi(\mathbf{r}, t) = 0$ preserve the Lorenz condition. All potentials in this restricted class are said to belong to the Lorenz gauge. The restricted transformations are of particular importance in the covariant description of near-field quantum electrodynamics; see Chaps. 16 and 29.

Physically, *all* electromagnetic fields in *classical* electrodynamics are generated by charged particles in some kind of motion. Therefore, the most general and physically acceptable solutions to (2.14) and (2.15) are

$$\mathbf{A}(\mathbf{r}, t) = \mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \mathbf{J}(\mathbf{r}', t') d^3 r' dt', \quad (2.16)$$

$$\phi(\mathbf{r}, t) = \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \rho(\mathbf{r}', t') d^3 r' dt', \quad (2.17)$$

where, with $\mathbf{r} - \mathbf{r}' = \mathbf{R}$, $R = |\mathbf{R}|$, and $t - t' = \tau$,

$$g(R, \tau) = \frac{1}{4\pi R} \delta\left(\frac{R}{c_0} - \tau\right), \quad (2.18)$$

δ being the Dirac delta function. The quantity $g(R, \tau)$ is the so-called retarded scalar (or Huygens) propagator, and the solutions in (2.16) and (2.17) are written in propagator form. The presence of the Dirac delta function in $g(R, \tau)$ allows one to carry out immediately the integrations over time in (2.16) and (2.17). Thus, one obtains in the Lorenz gauge

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\mathbf{J}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3 r', \quad (2.19)$$

$$\phi(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3 r'. \quad (2.20)$$

In the Lorenz gauge the potentials $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ at a given space($\mathbf{r}$)-time(t) point hence are related to the current, $\mathbf{J}(\mathbf{r}', t')$, and charge, $\rho(\mathbf{r}', t')$, densities prevailing at the various space ($\mathbf{r}'$) points at the earlier times

$$t' = t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}. \quad (2.21)$$

On the basis of (2.19) and (2.20) one might be tempted to claim that electromagnetic fields propagate through space with the speed c_0 . However one must remember that the potentials are not physically observable quantities, and that the results in (2.19) and (2.20) only hold in the Lorenz gauge.

By combining (2.5), (2.7), (2.19) and (2.20) one finally obtains the following *physically general* solution to the Maxwell–Lorentz equations:

$$\begin{aligned} \mathbf{E}(\mathbf{r}, t) = & -\frac{\partial}{\partial t} \left[\frac{1}{4\pi\epsilon_0 c_0^2} \int_{-\infty}^{\infty} \frac{\mathbf{J}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \right] \\ & - \nabla \left[\frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \right], \end{aligned} \quad (2.22)$$

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \left[\frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\mathbf{J}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \right]. \quad (2.23)$$

The results in (2.22) and (2.23) are of course gauge invariant but one *cannot* from these equations conclude that electromagnetic fields propagate through space with the speed c_0 , because these equations are not written in strict propagator form, and because the charge and current densities are not independent of each other but related via a local charge conservation condition; see Sect. 2.7.1. The possibilities of writing (2.22) and (2.23) in propagator form, and the problems one faces in the near-field zone of matter, and only here, are discussed in Chap. 3.

From a *mathematical* point of view the solutions to (2.19) and (2.20) represent *particular* solutions to the second-order partial differential equations in (2.14) and (2.15). To these solutions one may add (general) solutions to the homogeneous parts of the equations. Basically, such solutions have no physical importance because *all* fields in classical electrodynamics originate in some $(\mathbf{J}, \rho)$ -source. It is nevertheless true that solutions to the homogeneous wave equations may be of relevance in *certain* parts of space in *some* time interval. This is so because of the retardation effect. Sources electrostatically active for a finite time emit fields which may exist and propagate (with the speed of light) through empty space after the source has stopped its electrodynamic activity. The role of these free fields in the near-field zone of matter is quite complicated to describe, and we shall return to this issue in Chap. 14. The current and charge densities appearing in (2.16) and (2.17) are total quantities for matter in the entire space. In most cases one wants to investigate the dynamics of a particular set of charges located in what we call the system (syst) under study. Let us denote the charge and current densities of these by $\rho_{\text{syst}}(\mathbf{r}, t)$ and $\mathbf{J}_{\text{syst}}(\mathbf{r}, t)$, respectively. In electrodynamics we study the system dynamics by electromagnetic fields generated by another (distinguishable!) set of charges located in what we call the source (laser, lamp, near-field tip, etc. ...). We denote the associated charge and current densities by $\rho_{\text{source}}(\mathbf{r}, t)$ and $\mathbf{J}_{\text{source}}(\mathbf{r}, t)$. If no other charge distributions are present (of relevance), one has $\mathbf{J} = \mathbf{J}_{\text{source}} + \mathbf{J}_{\text{syst}}$, and $\rho = \rho_{\text{source}} + \rho_{\text{syst}}$. By insertion of these divisions into (2.19) and (2.20) one obtains

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_{\text{source}}(\mathbf{r}, t) + \frac{\mu_0}{4\pi} \int_{V_{\text{syst}}} \frac{\mathbf{J}_{\text{syst}}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3r', \quad (2.24)$$

$$\rho(\mathbf{r}, t) = \rho_{\text{source}}(\mathbf{r}, t) + \frac{1}{4\pi\epsilon_0} \int_{V_{\text{syst}}} \frac{\rho_{\text{syst}}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3r', \quad (2.25)$$

where the integration is over the domain, V_{syst} , of the system. The potentials

$$\mathbf{A}_{\text{source}}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int_{V_{\text{source}}} \frac{\mathbf{J}_{\text{source}}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3r', \quad (2.26)$$

$$\rho_{\text{source}}(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int_{V_{\text{source}}} \frac{\rho_{\text{source}}\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right)}{|\mathbf{r} - \mathbf{r}'|} d^3r', \quad (2.27)$$

are those generated by the source-particle dynamics, the integration being over the source volume, V_{source} . The source potentials may in certain regions of the space-time domain be freely propagating potentials, and, in case, appear as solutions to the homogeneous parts of the wave equations in (2.14) and (2.15).

The expressions for $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ in (2.22) and (2.23) have been characterized as the general *explicit* solution to the Maxwell–Lorentz equations. This is correct if the current and charge densities were *prescribed* quantities. To assume that $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ are prescribed entities is always an approximation, and in

most cases of interest such an approximation is too crude. In electrodynamics the time-dependent charge and current densities are generated by the local electromagnetic fields acting on them, and therefore (2.22) and (2.23) in a sense are *implicit* solutions to the Maxwell–Lorentz equations.

2.4 The Newton–Lorentz Equation

In the microscopic classical theory of electrodynamics it is assumed that the charged particles are point-particles. To the extent that the particle concept is meaningful, the elementary spin- $\frac{1}{2}$ fermions, leptons and quarks, are point particles without internal structure. In the present book mainly the electron (a charged lepton), proton and neutron are of interest. Although the proton and neutron are not point particles, it is usually sufficient to treat them as point-like quantities in microscopic electrodynamics. The proton consist of two up-quarks and one down-quark of charge $+\frac{2}{3}e$ and $-\frac{1}{3}e$ (e being the magnitude of the electron charge), and the neutron is build from one up-quark and two down-quarks [154–157].

In the point-particle description the charge and current densities are given by

$$\rho(\mathbf{r}, t) = \sum_{\alpha} q_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)), \quad (2.28)$$

$$\mathbf{J}(\mathbf{r}, t) = \sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)), \quad (2.29)$$

where q_{α} , $\mathbf{r}_{\alpha}(t)$ and $\mathbf{v}_{\alpha}(t) = d\mathbf{r}_{\alpha}(t)/dt$, denote the electrical charge, position, and velocity, respectively, of particle α . As before δ denote the Dirac delta function. The position and velocity of the various particles usually depend on time, as indicated, and the dynamics of particle α is described by the relativistic Newton–Lorentz equation [19, 130]

$$\frac{d}{dt} \mathbf{p}_{\alpha}(t) = q_{\alpha} [\mathbf{E}(\mathbf{r}_{\alpha}(t), t) + \mathbf{v}_{\alpha}(t) \times \mathbf{B}(\mathbf{r}_{\alpha}(t), t)], \quad (2.30)$$

where the relativistic momentum, $\mathbf{p}_{\alpha}(t)$, of the particle is given by

$$\mathbf{p}_{\alpha}(t) = \frac{m_{\alpha} \mathbf{v}_{\alpha}(t)}{\sqrt{1 - \left(\frac{v_{\alpha}(t)}{c_0}\right)^2}}, \quad (2.31)$$

m_{α} being the particle's rest mass, and $\mathbf{v}_{\alpha} \cdot \mathbf{v}_{\alpha} = v_{\alpha}^2$. In the nonrelativistic regime $\mathbf{p}_{\alpha}(t) = m_{\alpha} \mathbf{v}_{\alpha}(t)$.

The microscopic Maxwell–Lorentz equations ((2.1)–(2.4), with ρ and $\mathbf{J}$ given by (2.28) and (2.29)) plus the Newton–Lorentz equations for the various particles ((2.30) for particle α) form a set of selfconsistent equations for the dynamics of the global field–particle system.

2.5 The Liénard–Wiechert Potentials and Fields

In the point-particle approach to classical electrodynamics particularly simple expressions can be obtained for the scalar and vector potentials in the Lorenz gauge. To show this it is sufficient to consider the potentials from a single point-particle with charge Q , position $\mathbf{r}_Q(t)$, and velocity $\mathbf{v}_Q(t)$ at time t . By inserting the charge and current densities

$$\rho(\mathbf{r}, t) = Q\delta(\mathbf{r} - \mathbf{r}_Q(t)), \quad (2.32)$$

and

$$\mathbf{J}(\mathbf{r}, t) = Q\mathbf{v}_Q(t)\delta(\mathbf{r} - \mathbf{r}_Q(t)) \quad (2.33)$$

into (2.16) and (2.17) it is relatively easy to determine the potentials. Hence, let us first consider the calculation of the scalar potential. The presence of the delta function $\delta(\mathbf{r}' - \mathbf{r}_Q(t'))$ enables one to carry out the $\mathbf{r}'$ -integration immediately. Thus, with insertion of the explicit expression for the scalar propagator one obtains

$$\phi(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{1}{|\mathbf{r} - \mathbf{r}_Q(t')|} \delta\left(\frac{|\mathbf{r} - \mathbf{r}_Q(t')|}{c_0} - t + t'\right) dt'. \quad (2.34)$$

The integration over t' can be done provided we know the location $t' = t_r$ of the zero in the argument of the delta function. The time t_r is the solution to the equation

$$t_r = t - \frac{|\mathbf{r} - \mathbf{r}_Q(t_r)|}{c_0}. \quad (2.35)$$

The time t_r is called the retarded (r) time for obvious reasons, cf. (2.21). In principle, one cannot exclude the possibility that (2.35) has more than one solution, but in the following we assume that there is only one. If our system contains several particles one must solve an equation of the type in (2.35) for each particle. This is in general an impossible task because the trajectories of the various particles are determined by the electromagnetic fields generated by the other particles and the particles own field, in particular its self-field. In Sect. 7.4, we shall take up a brief discussion of the self-field problem for a point particle in the framework of classical electrodynamics. For a prescribed trajectory, (2.35) can relatively easily be solved by numerical methods, remembering that one has to solve the equation for each space($\mathbf{r}$)-time(t) point of interest. To carry out the t' -integration in (2.34), we make use of the mathematical result

$$\int_{-\infty}^{\infty} F(t')\delta(f(t')) dt' = \frac{F(t_r)}{|f'(t_r)|}, \quad (2.36)$$

valid under the assumption that $f(t')$ has one zero point (at $t' = t_r$). The quantity $f'(t_r)$ is the first derivative of $f(t')$ evaluated at $t' = t_r$. It is also assumed that $f'(t_r) \neq 0$. The result in (2.36) can be derived making a Taylor series expansion

of $f(t')$ around $t' = t_r$. Only the leading term in the series is needed, i.e., $f(t') = f'(t_r)(t' - t_r)$, since $f(t_r) = 0$. In the present case, where

$$f(t') = t' - t + \frac{|\mathbf{r} - \mathbf{r}_Q(t')|}{c_0} \quad (2.37)$$

a straightforward calculation gives

$$\frac{df(t')}{dt'} = 1 - \frac{1}{c_0} |\mathbf{r} - \mathbf{r}_Q(t')|^{-1} (\mathbf{r} - \mathbf{r}_Q(t')) \cdot \frac{d\mathbf{r}_Q(t')}{dt'}. \quad (2.38)$$

By combining (2.34), (2.36), and (2.38) one obtains

$$\phi(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \frac{1}{|\mathbf{r} - \mathbf{r}_Q(t_r)| - \frac{1}{c_0} \mathbf{v}_Q(t_r) \cdot (\mathbf{r} - \mathbf{r}_Q(t_r))}, \quad (2.39)$$

since $d\mathbf{r}_Q(t_r)/dt'_r = \mathbf{v}_Q(t_r)$. With the abbreviations

$$\mathbf{R}(t) = \mathbf{r} - \mathbf{r}_Q(t), \quad (2.40)$$

$$\boldsymbol{\beta}(t) = \frac{\mathbf{v}_Q(t)}{c_0}, \quad (2.41)$$

and the notation

$$\mathcal{F}(t_r) \equiv [\mathcal{F}]_{\text{ret}} \quad (2.42)$$

for the arbitrary function $\mathcal{F}$, the expression for the scalar potential in (2.39) can be written in the compact form

$$\phi(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \left[\frac{Q}{R(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})} \right]_{\text{ret}}, \quad (2.43)$$

where $R = |\mathbf{R}|$ and $\hat{\mathbf{R}} = \mathbf{R}/R$. A comparison of (2.17) and (2.32) to (2.16) and (2.33) readily shows that the vector potential of the point-particle is given by

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu_0 Q}{4\pi} \frac{\mathbf{v}_Q(t_r)}{|\mathbf{r} - \mathbf{r}_Q(t_r)| - \frac{1}{c_0} \mathbf{v}_Q(t_r) \cdot (\mathbf{r} - \mathbf{r}_Q(t_r))}, \quad (2.44)$$

cf (2.39), or in compact form as follows:

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \left[\frac{Q c_0 \boldsymbol{\beta}}{R(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})} \right]_{\text{ret}}. \quad (2.45)$$

In the Lorenz gauge, the scalar and vector potentials of a point particle thus are given by (2.43) and (2.45). These potentials are called the Liénard–Wiechert potentials, derived by Liénard in 1898, and independently by Wiechert 2 years later [158, 159].

In the nonrelativistic limit, $|\boldsymbol{\beta}| \ll 1$, the potentials reduce to the well known quasi-static forms, i.e., $\phi(\mathbf{r}, t) = Q/(4\pi\epsilon_0 R(t))$ and $\mathbf{A}(\mathbf{r}, t) = \mu_0 Q \mathbf{v}_Q(t)/(4\pi R(t))$, where $R(t)$ is the distance between the particle and observation point at the time t .

The electric and magnetic fields of the point particle now may be obtained inserting (2.43) and (2.45) into (2.5) and (2.7). Let us first calculate the time derivative of the vector potential. For this purpose we need the following results:

$$\frac{\partial \boldsymbol{\beta}(t_r)}{\partial t} = \frac{\partial t_r}{\partial t} \frac{\partial \boldsymbol{\beta}(t_r)}{\partial t_r} = \frac{\partial t_r}{\partial t} [\dot{\boldsymbol{\beta}}]_{\text{ret}}, \quad (2.46)$$

$$\frac{\partial R(t_r)}{\partial t} = \frac{\partial t_r}{\partial t} \frac{\partial R(t_r)}{\partial t_r} = -\frac{\partial t_r}{\partial t} \hat{\mathbf{R}}(t_r) \cdot \mathbf{v}_Q(t_r) = -\frac{\partial t_r}{\partial t} [c_0 \boldsymbol{\beta} \cdot \hat{\mathbf{R}}]_{\text{ret}}, \quad (2.47)$$

$$\frac{\partial \mathbf{R}(t_r)}{\partial t} = -\frac{\partial t_r}{\partial t} \mathbf{v}_Q(t_r) = -\frac{\partial t_r}{\partial t} [c_0 \boldsymbol{\beta}]_{\text{ret}}. \quad (2.48)$$

The quantity $\partial t_r / \partial t$ is obtained from (2.35). Hence,

$$\frac{\partial t_r}{\partial t} = 1 - \frac{1}{c_0} \frac{\partial R(t_r)}{\partial t} = 1 + \frac{\partial t_r}{\partial t} \boldsymbol{\beta}(t_r) \cdot \hat{\mathbf{R}}(t_r), \quad (2.49)$$

where (2.47) has been used to obtain the last equation, and then

$$\frac{\partial t_r}{\partial t} = \left[\frac{1}{1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}}} \right]_{\text{ret}} \quad (2.50)$$

in compact notation. By insertion of (2.50) into (2.46)–(2.48), the quantities $\partial \boldsymbol{\beta}(t_r) / \partial t$, $\partial R(t_r) / \partial t$, and $\partial \mathbf{R}(t_r) / \partial t$ are expressed completely as functions of the retarded time. To determine $-\partial \mathbf{A}(\mathbf{r}, t) / \partial t$ we utilize that

$$\frac{\partial}{\partial t} \left[\frac{\boldsymbol{\beta}}{R - \boldsymbol{\beta} \cdot \hat{\mathbf{R}}} \right]_{\text{ret}} = \left[\frac{R(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}}) \frac{\partial \boldsymbol{\beta}}{\partial t} - \boldsymbol{\beta} \left(\frac{\partial R}{\partial t} - \mathbf{R} \cdot \frac{\partial \boldsymbol{\beta}}{\partial t} - \boldsymbol{\beta} \cdot \frac{\partial \mathbf{R}}{\partial t} \right)}{R^2(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^2} \right]_{\text{ret}} \quad (2.51)$$

and insert in this equation the expressions in (2.46)–(2.49) (with (2.50)). A few elementary manipulations finally lead to

$$-\frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t} = -\frac{Q}{4\pi\epsilon_0} \left[\frac{c_0^{-1} \dot{\boldsymbol{\beta}}}{R(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^2} + \frac{\boldsymbol{\beta}(c_0^{-1} \dot{\boldsymbol{\beta}} \cdot \mathbf{R} + \boldsymbol{\beta} \cdot \hat{\mathbf{R}} - \beta^2)}{R^2(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^3} \right]_{\text{ret}}. \quad (2.52)$$

In order to calculate the gradient of the scalar potential one makes use of the following relations:

$$\nabla R(t_r) = \hat{\mathbf{R}}(t_r) - c_0 \boldsymbol{\beta}(t_r) \cdot \hat{\mathbf{R}}(t_r) \nabla t_r, \quad (2.53)$$

$$\nabla \boldsymbol{\beta}(t_r) = (\nabla t_r) \dot{\boldsymbol{\beta}}(t_r), \quad (2.54)$$

$$\nabla \mathbf{R}(t_r) = \mathbf{U} - c_0 (\nabla t_r) \boldsymbol{\beta}(t_r). \quad (2.55)$$

The last two equations are dyadic tensor relations, and $\mathbf{U}$ is the unit dyad (tensor) of dimension 3×3 . To express $\nabla R(t_r)$, $\nabla \boldsymbol{\beta}(t_r)$, and $\nabla \mathbf{R}(t_r)$ as functions of the retarded time we still need to find ∇t_r as a function of t_r . From (2.35), one obtains the implicit formula

$$\nabla t_r = -c_0^{-1} \hat{\mathbf{R}}(t_r) + \boldsymbol{\beta}(t_r) \cdot \hat{\mathbf{R}}(t_r) \nabla t_r \quad (2.56)$$

and hence

$$\nabla t_r = \left[\frac{c_0^{-1} \hat{\mathbf{R}}}{\boldsymbol{\beta} \cdot \hat{\mathbf{R}} - 1} \right]_{\text{ret}}. \quad (2.57)$$

It appears from (2.43) that to determine $\nabla \phi(\mathbf{r}, t)$ one needs an explicit expression for

$$\nabla \left[\frac{1}{R - \boldsymbol{\beta} \cdot \mathbf{R}} \right]_{\text{ret}} = \left[\frac{-\nabla R + (\nabla \boldsymbol{\beta}) \cdot \mathbf{R} + (\nabla \mathbf{R}) \cdot \boldsymbol{\beta}}{R^2(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^2} \right]_{\text{ret}}. \quad (2.58)$$

By inserting (2.53)–(2.55), and (2.57) into (2.58) one obtains after some elementary calculations

$$-\nabla \phi(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \left[\frac{\hat{\mathbf{R}}(1 - \beta^2 + c_0^{-1} \dot{\boldsymbol{\beta}} \cdot \mathbf{R}) - \boldsymbol{\beta}(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})}{R^2(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^3} \right]_{\text{ret}}. \quad (2.59)$$

A combination of (2.7), (2.52), and (2.59) finally gives the following relativistic result for the electric field of a point particle at the space-time point $(\mathbf{r}, t)$:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_{\text{vel}}(\mathbf{r}, t) + \mathbf{E}_{\text{acc}}(\mathbf{r}, t), \quad (2.60)$$

where

$$\mathbf{E}_{\text{vel}}(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \left[\frac{(1 - \beta^2)(\hat{\mathbf{R}} - \boldsymbol{\beta})}{R^2(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^3} \right]_{\text{ret}}, \quad (2.61)$$

and

$$\mathbf{E}_{\text{acc}}(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \left[\frac{\hat{\mathbf{R}} \times [(\hat{\mathbf{R}} - \boldsymbol{\beta}) \times \dot{\boldsymbol{\beta}}]}{c_0 R(1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}})^3} \right]_{\text{ret}}. \quad (2.62)$$

Above, the electric field has been divided into two parts, namely a so-called acceleration (acc) part, $\mathbf{E}_{\text{acc}}(\mathbf{r}, t)$, which is proportional to the particle acceleration at the retarded time, $\partial \boldsymbol{\beta}(t_r)/\partial t_r$, and a velocity (vel) part, $\mathbf{E}_{\text{vel}}(\mathbf{r}, t)$, which also is nonvanishing if the particle moves with uniform velocity. The distance between the point of observation $(\mathbf{r})$ at time t , and the position of the particle $(\mathbf{r}_Q)$ at the retarded time t_r , is R , and it appears from (2.61) and (2.62) that the velocity and acceleration fields vary with distance as R^{-2} and R^{-1} , respectively. The velocity field, which is also called the attached field, plays an important role in near-field electrodynamics as we realize later on. If the distance $R(t_r) = |\mathbf{r} - \mathbf{r}_Q(t_r)|$ is sufficiently large the acceleration field, also called the radiation field, dominates.

It appears from (2.52) and (2.59) that only the vector potential contributes to the R^{-1} -part of the field. Interference effects between the attached and radiation fields are of significance for the energy transport in the coupled matter–field system in near-field electrodynamics. If retardation effects are negligible, so that one formally can take the limit $c_0 \rightarrow \infty$, the electric field is given by the quasi-static expression $\mathbf{E}(\mathbf{r}, t) = Q \hat{\mathbf{R}}(t)/(4\pi\epsilon_0 R^2(t))$. In the electrostatic limit this is just the Coulomb field of a point charge. We shall discuss the near-field electrodynamics of a point charge in details later on.

The magnetic field of the relativistic point particle is obtained by combining (2.5) and (2.45). Since $\mathbf{A}(\mathbf{r}, t) = c_0^{-1}[\boldsymbol{\beta}\phi]_{\text{ret}}$, one has

$$c_0 \mathbf{B}(\mathbf{r}, t) = [\nabla\phi \times \boldsymbol{\beta}]_{\text{ret}} + [\phi \nabla \times \boldsymbol{\beta}]_{\text{ret}}. \quad (2.63)$$

From (2.54) and (2.57) it appears that the ij th component of $\nabla\boldsymbol{\beta}(t_r)$ is given by

$$(\nabla\boldsymbol{\beta}(t_r))_{ij} = \left[\frac{R_i \beta_j}{\boldsymbol{\beta} \cdot \hat{\mathbf{R}} - 1} \right]_{\text{ret}}, \quad (2.64)$$

when R_i is the i th Cartesian component of $\mathbf{R}$. A straightforward calculation then gives

$$[\nabla \times \boldsymbol{\beta}]_{\text{ret}} = -\frac{1}{c_0} \left[\frac{\hat{\mathbf{R}} \times \dot{\boldsymbol{\beta}}}{1 - \boldsymbol{\beta} \cdot \hat{\mathbf{R}}} \right]_{\text{ret}}. \quad (2.65)$$

The knowledge of $\phi(\mathbf{r}, t)$ (2.43), $\nabla\phi(\mathbf{r}, t)$ (2.59), and the expression for $[\nabla \times \boldsymbol{\beta}]_{\text{ret}}$ (2.65) easily leads to the following result for the magnetic field of our point charge:

$$\mathbf{B}(\mathbf{r}, t) = \mathbf{B}_{\text{vel}}(\mathbf{r}, t) + \mathbf{B}_{\text{acc}}(\mathbf{r}, t), \quad (2.66)$$

where the velocity (attached) part is given by

$$\mathbf{B}_{\text{vel}}(\mathbf{r}, t) = \frac{1}{c_0} [\hat{\mathbf{R}}]_{\text{ret}} \times \mathbf{E}_{\text{vel}}(\mathbf{r}, t) = \frac{1}{c_0} [\boldsymbol{\beta}]_{\text{ret}} \times \mathbf{E}_{\text{vel}}(\mathbf{r}, t), \quad (2.67)$$

and the acceleration (radiation) part by

$$\mathbf{B}_{\text{acc}}(\mathbf{r}, t) = \frac{1}{c_0} [\hat{\mathbf{R}}]_{\text{ret}} \times \mathbf{E}_{\text{acc}}(\mathbf{r}, t). \quad (2.68)$$

Equations (2.67) and (2.68) show that the distance ($R(t_r)$) dependences for $\mathbf{B}_{\text{vel}}(\mathbf{r}, t)$ and $\mathbf{B}_{\text{acc}}(\mathbf{r}, t)$ are the same as for the corresponding electric fields, and that both parts of the magnetic field are perpendicular to the direction from the particle position at the retarded time to the observation point at the present time. From (2.60), and (2.66)–(2.68) it appears that

$$c_0 \mathbf{B}(\mathbf{r}, t) = [\hat{\mathbf{R}}]_{\text{ret}} \times \mathbf{E}(\mathbf{r}, t). \quad (2.69)$$

In the quasi-stationary limit ($c_0 \rightarrow \infty$), one obtains combining (2.61) and (2.67) the well known magneto-static result $\mathbf{B} = \mu_0 Q \mathbf{v}_Q(t) \times \hat{\mathbf{R}}(t)/(4\pi R^2(t))$.

2.6 Some Important Global Conservation Laws

In this section, we shall show by explicit calculations that the total energy (H), the total momentum ($\mathbf{P}$), and the total angular momentum ($\mathbf{I}$) of the global system of particles plus electromagnetic field are constant in time. We expect these quantities to be conserved (constants of “the motion”) because the dynamical equations (the Maxwell–Lorentz and Newton–Lorentz equations) exhibit translational invariance in time and space, and rotational invariance in space.

Below, and throughout the book, we shall occasionally have to deal with bilinear expressions in various vector fields. For a generally complex field V , with complex conjugate V^* we shall use the following notation for the relevant bilinear expressions

$$V \cdot V^* = |V|^2, \quad (2.70)$$

$$V \cdot V = V^2. \quad (2.71)$$

2.6.1 Global Energy Conservation

The Coulomb energy of a system of electrically charged particles, consisting of the sum of the Coulomb interaction energy between the various pairs of particles plus the Coulomb self-energy of the individual particles, can be represented as a part of the energy stored in the electromagnetic field, viz., the energy contribution from the rotational-free (longitudinal) electric field to the field energy. The longitudinal electric field plays an important role in near-field electrodynamics as we shall realize later on. By inclusion of the Coulomb energy of the particle system as a part of the field energy, the remaining energy of the particles, H_{par} , is given by the relativistic expression [19, 116, 130, 144, 160]

$$H_{\text{par}} = c_0^2 \sum_{\alpha} m_{\alpha} \gamma_{\alpha}, \quad (2.72)$$

where

$$\gamma_{\alpha} = (1 - \beta_{\alpha}^2)^{-\frac{1}{2}}, \quad (2.73)$$

with

$$\beta_{\alpha} = \frac{v_{\alpha}}{c_0}. \quad (2.74)$$

The kinetic energy of the particle system is given by $H_{\text{par}} - c_0^2 \sum_{\alpha} m_{\alpha}$, where $c_0^2 \sum_{\alpha} m_{\alpha}$ is the rest energy of the particle system. The energy of the

electromagnetic field, H_{field} , is given by

$$H_{\text{field}} = \frac{1}{2} \epsilon_0 \int_{-\infty}^{\infty} (\mathbf{E}^2(\mathbf{r}, t) + c_0^2 \mathbf{B}^2(\mathbf{r}, t)) d^3r, \quad (2.75)$$

where, as indicated, the integration extends over the entire space. The total energy, H , of the global field–particle system thus is given by

$$H = H_{\text{par}} + H_{\text{field}}. \quad (2.76)$$

Due to the electrodynamic interaction with the field the particle energy changes in time, and since

$$\frac{d\gamma_\alpha}{dt} = c_0^{-2} \gamma_\alpha^3 \mathbf{v}_\alpha \cdot \frac{d\mathbf{v}_\alpha}{dt}, \quad (2.77)$$

one obtains

$$\frac{dH_{\text{par}}}{dt} = \sum_{\alpha} m_{\alpha} \gamma_{\alpha}^3 \mathbf{v}_{\alpha} \cdot \frac{d\mathbf{v}_{\alpha}}{dt}. \quad (2.78)$$

The right side of (2.78) also appears as follows:

$$\begin{aligned} \sum_{\alpha} \mathbf{v}_{\alpha} \cdot \frac{d}{dt} (\gamma_{\alpha} m_{\alpha} \mathbf{v}_{\alpha}) &= \sum_{\alpha} m_{\alpha} \mathbf{v}_{\alpha} \cdot \left(\mathbf{v}_{\alpha} \frac{d\gamma_{\alpha}}{dt} + \gamma_{\alpha} \frac{d\mathbf{v}_{\alpha}}{dt} \right) \\ &= \sum_{\alpha} m_{\alpha} \gamma_{\alpha}^3 \mathbf{v}_{\alpha} \cdot \frac{d\mathbf{v}_{\alpha}}{dt}, \end{aligned} \quad (2.79)$$

where the last relation is obtained by means of (2.77). By using the relativistic Newton–Lorentz equation in (2.30) in the first expression in (2.79) one gets

$$\sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha} \cdot \mathbf{E}(\mathbf{r}_{\alpha}(t), t) = \sum_{\alpha} m_{\alpha} \gamma_{\alpha}^3 \mathbf{v}_{\alpha} \cdot \frac{d\mathbf{v}_{\alpha}}{dt}, \quad (2.80)$$

since $\mathbf{v}_{\alpha} \cdot \mathbf{v}_{\alpha} \times \mathbf{B}(\mathbf{r}_{\alpha}(t), t) = 0$. A combination of (2.78) and (2.80) leads to

$$\frac{dH_{\text{par}}}{dt} = \sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha}(t) \cdot \mathbf{E}(\mathbf{r}_{\alpha}(t), t). \quad (2.81)$$

The increase of the particle energy, H_{par} , per unit time hence equals the sum of the works carried out by the electric field on the individual charges, as expected. The rate of change in the field energy, viz.,

$$\frac{dH_{\text{field}}}{dt} = \epsilon_0 \int_{-\infty}^{\infty} \left(\mathbf{E}(\mathbf{r}, t) \cdot \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} + c_0^2 \mathbf{B}(\mathbf{r}, t) \cdot \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} \right) d^3r, \quad (2.82)$$

can be written also as

$$\begin{aligned} \frac{dH_{\text{field}}}{dt} = \epsilon_0 \int_{-\infty}^{\infty} [& \mathbf{E}(\mathbf{r}, t) \cdot (c_0^2 \nabla \times \mathbf{B}(\mathbf{r}, t) - \epsilon_0^{-1} \mathbf{J}(\mathbf{r}, t)) \\ & - c_0^2 \mathbf{B}(\mathbf{r}, t) \cdot \nabla \times \mathbf{E}(\mathbf{r}, t)] d^3r, \end{aligned} \quad (2.83)$$

using the Maxwell–Lorentz equations in (2.1) and (2.3) to eliminate $\partial \mathbf{E} / \partial t$ and $\partial \mathbf{B} / \partial t$ from (2.82). The expression in (2.29) for the point-particle current density shows that

$$\int_{-\infty}^{\infty} \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{J}(\mathbf{r}, t) d^3r = \sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha}(t) \cdot \mathbf{E}(\mathbf{r}_{\alpha}(t), t), \quad (2.84)$$

and since $\nabla \cdot (\mathbf{E} \times \mathbf{B}) = \mathbf{B} \cdot \nabla \times \mathbf{E} - \mathbf{E} \cdot \nabla \times \mathbf{B}$, a combination of (2.76), (2.81), and (2.83), therefore, gives

$$\frac{dH}{dt} = - \int_{-\infty}^{\infty} \nabla \cdot (\mu_0^{-1} \mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r. \quad (2.85)$$

By applying Gauss’ theorem the volume integral can be transformed into a surface integral. Under the assumption that all the charges (in the universe) are located in a finite region of space, the integral over a surface infinitely far from a globally neutral charge distribution will be zero; see Chap. 5. We have thus proved the global conservation law

$$\frac{dH}{dt} = 0 \quad (2.86)$$

for the energy of the particle–field system.

2.6.2 Global Momentum Conservation

The total momentum, $\mathbf{P}$, of the global field–particle system, given by

$$\mathbf{P} = \mathbf{P}_{\text{par}} + \mathbf{P}_{\text{field}}, \quad (2.87)$$

where

$$\mathbf{P}_{\text{par}} = \sum_{\alpha} \gamma_{\alpha} m_{\alpha} \mathbf{v}_{\alpha} \quad (2.88)$$

is the relativistic momentum of all the particles, and

$$\mathbf{P}_{\text{field}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t) d^3r \quad (2.89)$$

is the momentum of the electromagnetic field, also is a conserved quantity. The field–matter interaction changes the relativistic momentum of the particle system at a rate

$$\frac{d\mathbf{P}_{\text{par}}}{dt} = \sum_{\alpha} \frac{d\mathbf{p}_{\alpha}(t)}{dt} = \sum_{\alpha} q_{\alpha} [\mathbf{E}(\mathbf{r}_{\alpha}(t), t) + \mathbf{v}_{\alpha}(t) \times \mathbf{B}(\mathbf{r}_{\alpha}(t), t)], \quad (2.90)$$

cf. the Newton–Lorentz equation in (2.30), and the field momentum at a rate

$$\frac{d\mathbf{P}_{\text{field}}}{dt} = \epsilon_0 \int_{-\infty}^{\infty} \left(\frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} \times \mathbf{B}(\mathbf{r}, t) + \mathbf{E}(\mathbf{r}, t) \times \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} \right) d^3r. \quad (2.91)$$

By using the Maxwell–Lorentz equations (2.1) and (2.3) to eliminate $\partial \mathbf{B} / \partial t$ and $\partial \mathbf{E} / \partial t$, (2.91) takes the form

$$\begin{aligned} \frac{d\mathbf{P}_{\text{field}}}{dt} = & - \int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t) d^3r \\ & - \int_{-\infty}^{\infty} \left[\frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \times (\nabla \times \mathbf{B}(\mathbf{r}, t)) + \epsilon_0 \mathbf{E}(\mathbf{r}, t) \times (\nabla \times \mathbf{E}(\mathbf{r}, t)) \right] d^3r. \end{aligned} \quad (2.92)$$

To show that the sum of $d\mathbf{P}_{\text{par}}/dt$ and $d\mathbf{P}_{\text{field}}/dt$ is zero one uses a certain tensor identity to rewrite the last integral in (2.92). Thus, for a general vector(field) $\mathbf{V}$ one has

$$\mathbf{V} \times (\nabla \times \mathbf{V}) = (\nabla \mathbf{V}) \cdot \mathbf{V} - (\mathbf{V} \cdot \nabla) \mathbf{V}, \quad (2.93)$$

$$(\nabla \mathbf{V}) \cdot \mathbf{V} = \frac{1}{2} \nabla (\mathbf{V} \cdot \mathbf{V}), \quad (2.94)$$

$$(\mathbf{V} \cdot \nabla) \mathbf{V} = \nabla \cdot (\mathbf{V} \mathbf{V}) - (\nabla \cdot \mathbf{V}) \mathbf{V}, \quad (2.95)$$

and hence

$$\mathbf{V} \times (\nabla \times \mathbf{V}) = \frac{1}{2} \nabla (\mathbf{V} \cdot \mathbf{V}) - \nabla \cdot (\mathbf{V} \mathbf{V}) + (\nabla \cdot \mathbf{V}) \mathbf{V}. \quad (2.96)$$

The Maxwell–Lorentz equations in (2.2) and (2.4) imply that the last term in (2.96) equals $\rho \mathbf{E} / \epsilon_0$ for $\mathbf{V} = \mathbf{E}$, and is zero for $\mathbf{V} = \mathbf{B}$. Altogether, (2.92) may therefore be written as follows:

$$\begin{aligned} \frac{d\mathbf{P}_{\text{field}}}{dt} = & - \int_{-\infty}^{\infty} (\rho(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r \\ & + \int_{-\infty}^{\infty} \left[\nabla \cdot \left(\epsilon_0 \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t) \right) \right. \\ & \left. - \frac{1}{2} \nabla \left(\epsilon_0 \mathbf{E}(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \mathbf{B}(\mathbf{r}, t) \right) \right] d^3r. \end{aligned} \quad (2.97)$$

By insertion of the point-particle expressions for the charge and current densities ((2.28) and (2.29)) the first integral in (2.97) can be determined. Thus,

$$\begin{aligned} \int_{-\infty}^{\infty} (\rho(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r \\ = \sum_{\alpha} q_{\alpha} [\mathbf{E}(\mathbf{r}_{\alpha}(t), t) + \mathbf{v}_{\alpha}(t) \times \mathbf{B}(\mathbf{r}_{\alpha}(t), t)]. \end{aligned} \quad (2.98)$$

By combining (2.87), (2.90), (2.97), and (2.98), and using the relation

$$\nabla V = \nabla \cdot (\mathbf{U} V) \quad (2.99)$$

for the scalar field V , it appears that

$$\begin{aligned} \frac{d\mathbf{P}}{dt} = \int_{-\infty}^{\infty} \nabla \cdot \left[\epsilon_0 \mathbf{E}(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \mathbf{B}(\mathbf{r}, t) \right. \\ \left. - \frac{1}{2} \mathbf{U} \left(\epsilon_0 \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t) \right) \right] d^3r. \end{aligned} \quad (2.100)$$

By means of Gauss' theorem the volume integral can be transformed into a surface integral over a surface infinitely far from the charge distribution. Since this surface integral vanishes, the global conservation law

$$\frac{d\mathbf{P}}{dt} = \mathbf{0} \quad (2.101)$$

for the total momentum of the particle–field system is proved.

2.6.3 Global Angular Momentum Conservation

The total angular momentum, $\mathbf{I}$, of the global field–particle system is given by the sum

$$\mathbf{I} = \mathbf{I}_{\text{par}} + \mathbf{I}_{\text{field}} \quad (2.102)$$

of the relativistic angular momentum of the particles,

$$\mathbf{I}_{\text{par}} = \sum_{\alpha} \mathbf{r}_{\alpha} \times \mathbf{p}_{\alpha}, \quad (2.103)$$

with $\mathbf{p}_{\alpha}$ given by (2.31), and the angular momentum of the electromagnetic field,

$$\mathbf{I}_{\text{field}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{r} \times (\mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r. \quad (2.104)$$

A calculation quite similar to the one carried out for the momentum of the particle–field system leads to the result

$$\begin{aligned} \frac{d\mathbf{I}}{dt} = \int_{-\infty}^{\infty} \mathbf{r} \times \nabla \cdot \left[\epsilon_0 \mathbf{E}(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \mathbf{B}(\mathbf{r}, t) \right. \\ \left. - \frac{1}{2} U \left(\epsilon_0 \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) + \frac{1}{\mu_0} \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t) \right) \right] d^3r. \end{aligned} \quad (2.105)$$

Again, the volume integral on the right side of (2.105) can be replaced by a certain surface integral (see Sect. 2.7), and since this surface integral over a surface infinitely far from the point-particles vanishes, the global conservation law,

$$\frac{d\mathbf{I}}{dt} = \mathbf{0} \quad (2.106)$$

for the total angular momentum of the particle–field system appears.

2.7 Some Local Conservation Laws

2.7.1 Charge Conservation

Inherent in the Maxwell–Lorentz equations one has an equation of continuity which expresses the local conservation of the global electric charge. The equation of continuity is obtained by taking first the divergence of (2.3). Since $\nabla \cdot \nabla \times \mathbf{B}(\mathbf{r}, t) = 0$ this gives

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \epsilon_0 \frac{\partial}{\partial t} \nabla \cdot \mathbf{E}(\mathbf{r}, t) = 0, \quad (2.107)$$

remembering that $\epsilon_0 \mu_0 = c_0^{-2}$. Using (2.2) to eliminate $\nabla \cdot \mathbf{E}(\mathbf{r}, t)$ one then obtains

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \frac{\partial}{\partial t} \rho(\mathbf{r}, t) = 0, \quad (2.108)$$

i.e., the equation of continuity for the charge. In the point-particle description, the charge and current densities are given by (2.28) and (2.29). Since

$$\begin{aligned} \nabla \cdot \mathbf{J}(\mathbf{r}, t) &= \sum_{\alpha} q_{\alpha} \nabla \cdot [\mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t))] = \sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha}(t) \cdot \nabla \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \\ &= - \sum_{\alpha} q_{\alpha} \mathbf{v}_{\alpha}(t) \cdot \nabla_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)), \end{aligned} \quad (2.109)$$

where ∇_α is the gradient with respect to $\mathbf{r}_\alpha$, and

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) = \sum_\alpha q_\alpha \frac{\partial}{\partial t} \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) = \sum_\alpha q_\alpha \mathbf{v}_\alpha \cdot \nabla_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) \quad (2.110)$$

using the chain rule $\partial/\partial t = \mathbf{v}_\alpha \cdot \nabla_\alpha$, it appears that the point-particle expressions for $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ indeed satisfy the equation of continuity. One may elaborate a bit on the point-particle charge conservation by integrating the two terms in (2.108) over a fixed (in time) volume V enclosed by the surface S . By means of one of Gauss's theorems integration of the first term in (2.108) gives

$$\begin{aligned} \int_V \nabla \cdot \mathbf{J}(\mathbf{r}, t) dV &= \oint_S \mathbf{J}(\mathbf{r}, t) \cdot d\mathbf{S} \\ &= \sum_\alpha q_\alpha \mathbf{v}_\alpha(t) \cdot \oint_S \hat{\mathbf{n}}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) dS, \end{aligned} \quad (2.111)$$

where $\hat{\mathbf{n}}$ is an outwards directed unit normal vector for the surface element dS , i.e., $d\mathbf{S} = \hat{\mathbf{n}} dS$. The current density flux through S thus is zero at time t , unless one (or more) particle(s) is(are) located somewhere on S at this time. Integration of the second term in (2.108) gives

$$\frac{d}{dt} \int_V \rho(\mathbf{r}, t) dV = \frac{d}{dt} \sum_\alpha q_\alpha \int_V \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) dV = \frac{dQ(t)}{dt}, \quad (2.112)$$

where $Q(t)$ is the total charge of those particles which happen to be inside the volume V at time t . This charge changes in a step-function like manner (step height q_i when a particular particle (number i) passes the surface S).

2.7.2 Local Energy Conservation: Microscopic Poynting Vector

Let us now introduce two quantities, which at least in classical electrodynamics make some sense, namely, the microscopic energy density in the electromagnetic field

$$W(\mathbf{r}, t) = \frac{1}{2} \epsilon_0 (\mathbf{E}^2(\mathbf{r}, t) + c_0^2 \mathbf{B}^2(\mathbf{r}, t)), \quad (2.113)$$

and the microscopic Poynting vector of the field

$$\mathbf{S}(\mathbf{r}, t) = \frac{1}{\mu_0} \mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t). \quad (2.114)$$

In Sect. 2.6.1, we obtained (2.85) by integrating over the entire space. It is obvious, however, that if one instead integrates over a finite (fixed) volume V one gets

$$\int_V \frac{\partial}{\partial t} W(\mathbf{r}, t) d^3r + \frac{d}{dt} H_{\text{par}}(\alpha \in V) = - \int_V \nabla \cdot \mathbf{S}(\mathbf{r}, t) d^3r, \quad (2.115)$$

where $H_{\text{par}}(\alpha \in V)$ means that only those particles which are inside V at time t are included in the particle energy. It appears from (2.81) that $dH_{\text{par}}(\alpha \in V)/dt$ can be rewritten as an integral over V . Thus,

$$\begin{aligned} \frac{d}{dt} H_{\text{par}}(\alpha \in V) &= \sum_{\alpha \in V} q_\alpha v_\alpha(t) \cdot \mathbf{E}(\mathbf{r}_\alpha(t), t) \\ &= \int_V \left[\sum_{\alpha} q_\alpha v_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) \right] \cdot \mathbf{E}(\mathbf{r}, t) d^3r. \end{aligned} \quad (2.116)$$

Note that the delta function $\delta(\mathbf{r} - \mathbf{r}_\alpha(t))$ automatically ensures that only particles inside V at time t contribute. Since the volume V is arbitrary, (2.115) (with (2.116) inserted) can be cast into the form of a differential energy conservation law, viz.,

$$- \frac{\partial W(\mathbf{r}, t)}{\partial t} = \left[\sum_{\alpha} q_\alpha v_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha(t)) \right] \cdot \mathbf{E}(\mathbf{r}, t) + \nabla \cdot \mathbf{S}(\mathbf{r}, t). \quad (2.117)$$

When (2.117) is integrated over a volume, v , which does not contain any particles, one obtains

$$- \frac{d}{dt} \int_v W(\mathbf{r}, t) d^3r = \int_v \nabla \cdot \mathbf{S}(\mathbf{r}, t) d^3r = \oint_s \mathbf{S}(\mathbf{r}, t) \cdot \hat{\mathbf{n}} ds, \quad (2.118)$$

an equation which expresses the fact that the rate of loss of electromagnetic energy in v equals the rate at which net energy is flowing out of v through the enclosing surface s , $\mathbf{S}(\mathbf{r}, t)$ representing the local electromagnetic energy flow (energy/area $\times$ time). If there happens to be one (or more) particle(s) in v at time t part of the field energy loss in v is used to increase the relativistic kinetic (kin) energy of the particle(s)

$$H_{\text{par}}^{\text{kin}}(\alpha \in V) = H_{\text{par}}(\alpha \in v) - c_0^2 \sum_{\alpha \in v} m_\alpha, \quad (2.119)$$

at a rate $dH_{\text{par}}^{\text{kin}}/dt = dH_{\text{par}}/dt$ given by (2.78); cf. (2.80).

2.7.3 Local Momentum Conservation: Maxwell Stress Tensor

The expression for the field momentum in (2.89) makes it natural to consider

$$\mathbf{g}(\mathbf{r}, t) = \epsilon_0 \mathbf{E}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t) = c_0^{-2} \mathbf{S}(\mathbf{r}, t) \quad (2.120)$$

as the momentum density of the electromagnetic field. Introducing also the so-called Maxwell stress tensor [19, 116, 130, 144]

$$\begin{aligned} \mathbf{T} = & \epsilon_0 \mathbf{E}(\mathbf{r}, t) \mathbf{E}(\mathbf{r}, t) + \mu_0^{-1} \mathbf{B}(\mathbf{r}, t) \mathbf{B}(\mathbf{r}, t) \\ & - \frac{1}{2} \mathbf{U} \left(\epsilon_0 \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) + \mu_0^{-1} \mathbf{B}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t) \right), \end{aligned} \quad (2.121)$$

a symmetric tensor, written here in dyadic form, one obtains (in analogy with (2.100)) if the integration is over an arbitrary finite (fixed) volume V the result

$$\int_V \frac{\partial}{\partial t} \mathbf{g}(\mathbf{r}, t) d^3r + \frac{d}{dt} \mathbf{P}_{\text{par}}(\alpha \in V) = \int_V \nabla \cdot \mathbf{T}(\mathbf{r}, t) d^3r. \quad (2.122)$$

Since

$$\mathbf{P}_{\text{par}}(\alpha \in V) = \int_V \sum_{\alpha} \gamma_{\alpha}(t) m_{\alpha} \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) d^3r \quad (2.123)$$

the differential form of (2.122) is

$$-\frac{\partial \mathbf{g}(\mathbf{r}, t)}{\partial t} = \frac{\partial}{\partial t} \sum_{\alpha} \gamma_{\alpha}(t) m_{\alpha} \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) + \nabla \cdot (-\mathbf{T}(\mathbf{r}, t)). \quad (2.124)$$

A clear picture of the physics hidden in (2.124) emerges if one rewrites the particle term as follows:

$$\begin{aligned} \frac{\partial}{\partial t} \sum_{\alpha} \mathbf{p}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \\ = \sum_{\alpha} \left[\delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d\mathbf{p}_{\alpha}(t)}{dt} - \mathbf{p}_{\alpha}(t) \mathbf{v}_{\alpha}(t) \cdot \nabla \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \right], \end{aligned} \quad (2.125)$$

and thereafter uses in the last term the tensor relation

$$\nabla \cdot (\mathbf{A} \mathbf{B}) = (\nabla \cdot \mathbf{A}) \mathbf{B} + (\mathbf{A} \cdot \nabla) \mathbf{B} \quad (2.126)$$

with $\mathbf{A} = \delta \mathbf{v}_{\alpha}$ and $\mathbf{B} = \mathbf{p}_{\alpha}$. Since $\mathbf{p}_{\alpha}$ is independent of $\mathbf{r}$ one obtains

$$\nabla \cdot (\delta \mathbf{v}_{\alpha} \mathbf{p}_{\alpha}) = [\nabla \cdot (\delta \mathbf{v}_{\alpha})] \mathbf{p}_{\alpha} = \mathbf{p}_{\alpha} \nabla \cdot (\delta \mathbf{v}_{\alpha}) = \mathbf{p}_{\alpha} \mathbf{v}_{\alpha} \cdot \nabla \delta, \quad (2.127)$$

and hence

$$\begin{aligned} \frac{\partial}{\partial t} \sum_{\alpha} \mathbf{p}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) = \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d\mathbf{p}_{\alpha}(t)}{dt} \\ - \nabla \cdot \left[\sum_{\alpha} \gamma_{\alpha} m_{\alpha} \mathbf{v}_{\alpha}(t) \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \right]. \end{aligned} \quad (2.128)$$

By inserting (2.128) into (2.124) one finally has

$$-\frac{\partial \mathbf{g}(\mathbf{r}, t)}{\partial t} = \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d\mathbf{p}_{\alpha}(t)}{dt} + \nabla \cdot \mathbf{S}(\mathbf{r}, t), \quad (2.129)$$

where

$$\mathbf{S}(\mathbf{r}, t) = -\mathbf{T}(\mathbf{r}, t) - \sum_{\alpha} \gamma_{\alpha}(t) m_{\alpha} \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \quad (2.130)$$

is the (symmetric) stress tensor of the particle–field system. Equation (2.129) is the local momentum conservation law, which upon integration over a volume v shows that the rate of loss of field momentum in v equals the rate of momentum increase in the particles within v plus the rates of field $[\nabla \cdot (-\mathbf{T})]$ and particle $[\nabla \cdot (\mathbf{S} + \mathbf{T})]$ momentum flow out of v . If the volume v does not contain any particles, the equation

$$-\frac{d}{dt} \int_v \mathbf{g}(\mathbf{r}, t) d^3r = \oint_s \mathbf{T}(\mathbf{r}, t) \cdot \hat{\mathbf{n}}(\mathbf{r}) ds \quad (2.131)$$

represents the momentum conservation of the free electromagnetic field.

2.7.4 Local Angular Momentum Conservation: Angular Momentum Flow

The results in (2.105) in a sense represents the global angular momentum conservation. If one assumes in the calculation leading up to this equation that the integration volume V is finite (and fixed) one obtains the balance equation

$$\int_V \frac{\partial}{\partial t} (\mathbf{r} \times \mathbf{g}(\mathbf{r}, t)) d^3r + \frac{d}{dt} \mathbf{I}_{\text{par}}(\alpha \in V) = \int_V \mathbf{r} \times \nabla \cdot \mathbf{T}(\mathbf{r}, t) d^3r \quad (2.132)$$

for the angular momentum of the particle–field system. On differential form (2.132) becomes

$$-\frac{\partial}{\partial t} (\mathbf{r} \times \mathbf{g}(\mathbf{r}, t)) = \frac{\partial}{\partial t} \sum_{\alpha} \mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) - \mathbf{r} \times \nabla \cdot \mathbf{T}(\mathbf{r}, t). \quad (2.133)$$

The particle term can be transformed in a manner analogous to the one employed in Sect. 2.7.3. Doing this we get

$$\begin{aligned} -\frac{\partial}{\partial t} (\mathbf{r} \times \mathbf{g}(\mathbf{r}, t)) &= \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d}{dt} (\mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t)) \\ &\quad - \nabla \cdot \left[\sum_{\alpha} \mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t) \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \right] - \mathbf{r} \times \nabla \cdot \mathbf{T}(\mathbf{r}, t). \end{aligned} \quad (2.134)$$

The last term in (2.134) can be replaced by the divergence of the tensorfield $-\mathbf{T} \times \mathbf{r}$. In order to prove this one may use the following tensor relations:

$$\nabla \cdot (\mathbf{A}\mathbf{B} \times \mathbf{r}) = (\nabla \cdot \mathbf{A})(\mathbf{B} \times \mathbf{r}) + (\mathbf{A} \cdot \nabla)(\mathbf{B} \times \mathbf{r}), \quad (2.135)$$

$$(\mathbf{A} \cdot \nabla)(\mathbf{B} \times \mathbf{r}) = [(\mathbf{A} \cdot \nabla)\mathbf{B}] \times \mathbf{r} - \mathbf{A} \cdot \nabla \mathbf{r} \times \mathbf{B}. \quad (2.136)$$

Since $\nabla \mathbf{r} = \mathbf{U}$ and $\mathbf{A} \cdot \mathbf{U} \times \mathbf{B} = \mathbf{A} \times \mathbf{B}$, combination of (2.135) and (2.136) gives

$$\nabla \cdot (\mathbf{A}\mathbf{B} \times \mathbf{r}) = -\mathbf{r} \times (\nabla \cdot \mathbf{A})\mathbf{B} - \mathbf{r} \times (\mathbf{A} \cdot \nabla)\mathbf{B} - \mathbf{A} \times \mathbf{B}, \quad (2.137)$$

and hence with the help of (2.126)

$$\nabla \cdot (\mathbf{A}\mathbf{B} \times \mathbf{r}) = -\mathbf{r} \times \nabla \cdot (\mathbf{A}\mathbf{B}) - \mathbf{A} \times \mathbf{B}. \quad (2.138)$$

Application of (2.138) to the symmetric stress tensor in (2.121) readily leads to the desired result

$$\nabla \cdot (\mathbf{T} \times \mathbf{r}) = -\mathbf{r} \times \nabla \cdot \mathbf{T} \quad (2.139)$$

since $\mathbf{A} \times \mathbf{B} = 0$ for $\mathbf{A} = \mathbf{B}$. On differential form the local angular momentum conservation law therefore takes the form

$$-\frac{\partial}{\partial t}(\mathbf{r} \times \mathbf{g}(\mathbf{r}, t)) = \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d}{dt}(\mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t)) + \nabla \cdot \mathcal{M}(\mathbf{r}, t), \quad (2.140)$$

where

$$\mathcal{M}(\mathbf{r}, t) = \mathbf{T}(\mathbf{r}, t) \times \mathbf{r} - \sum_{\alpha} \gamma_{\alpha}(t) m_{\alpha} \mathbf{r}_{\alpha}(t) \times \mathbf{v}_{\alpha}(t) \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)). \quad (2.141)$$

Equations (2.140) and (2.141) show after integration over a volume v that the rate of angular momentum loss in v is balanced by the rate of increase in the angular momentum of the particles inside v plus the rates of field and particle angular momentum flow out of v . If there are no particles in v the relation

$$-\frac{d}{dt} \int_v \mathbf{r} \times \mathbf{g}(\mathbf{r}, t) d^3r = \oint_s \mathbf{T}(\mathbf{r}, t) \times \mathbf{r} \cdot \hat{\mathbf{n}}(\mathbf{r}) ds \quad (2.142)$$

expresses the angular momentum conservation of the free electromagnetic field.

Chapter 3

Electromagnetic Green Functions in Spectral Representation

3.1 The Maxwell–Lorentz Equations in the Space–Frequency Domain

A spectral representation of the Maxwell–Lorentz equations can be obtained subjecting the various vector fields ($\mathbf{E}$, $\mathbf{B}$, and $\mathbf{J}$) and the scalar field (ρ) to a timely Fourier integral transformation. For a vector field $\mathbf{V}$ the transformation is defined by

$$\mathbf{V}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \mathbf{V}(\mathbf{r}, t) e^{i\omega t} dt, \quad (3.1)$$

and for a scalar field the transformation is the same as for a component of $\mathbf{V}$. Since all the fields in the Maxwell–Lorentz equations are real it is required that

$$\mathbf{V}(\mathbf{r}; -\omega) = \mathbf{V}^*(\mathbf{r}; \omega), \quad (3.2)$$

where $*$ means complex conjugation. The inverse transformation to (3.1) is

$$\mathbf{V}(\mathbf{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{V}(\mathbf{r}; \omega) e^{-i\omega t} d\omega. \quad (3.3)$$

It readily appears from (3.3) that the Fourier transform of $\partial \mathbf{V}(\mathbf{r}, t)/\partial t$ is $-i\omega \mathbf{V}(\mathbf{r}; \omega)$, so that differentiation in time in the time domain is replaced by multiplication by $-i\omega$ in the spectral domain, in the following called the angular frequency (ω) domain or for brevity just the frequency domain. In operator notation we thus have the prescription

$$\frac{\partial}{\partial t} \Leftrightarrow -i\omega. \quad (3.4)$$

In the space($\mathbf{r}$)–frequency(ω) domain the microscopic Maxwell–Lorentz equations in (2.1)–(2.4) therefore take the following forms:

$$\nabla \times \mathbf{E}(\mathbf{r}; \omega) = i\omega \mathbf{B}(\mathbf{r}; \omega), \quad (3.5)$$

$$\nabla \cdot \mathbf{E}(\mathbf{r}; \omega) = \frac{1}{\epsilon_0} \rho(\mathbf{r}; \omega), \quad (3.6)$$

$$\nabla \times \mathbf{B}(\mathbf{r}; \omega) = \mu_0 \mathbf{J}(\mathbf{r}; \omega) - \frac{i\omega}{c_0^2} \mathbf{E}(\mathbf{r}; \omega), \quad (3.7)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}; \omega) = 0. \quad (3.8)$$

For a given problem the (approximate) solution of the Maxwell–Lorentz equations is often easier to obtain in the space–frequency domain than in the space–time domain because differentiation in time is replaced by simple multiplication, cf. the prescription in (3.4). Once the solution has been obtained to (3.5)–(3.8) the general time dependence of the various vector and scalar fields can be obtained from (3.3).

3.2 Dyadic Green Functions in the Space–Frequency Domain

3.2.1 Green Function for the Electric Field

In Sect. 2.3, integral relations in space–time were established between the vector potential and the particle current density (2.16), and between the scalar potential and the charge density (2.17). The two integrals have the same kernel, namely the Huygens propagator (2.18), and the integrals are folding integrals in both space and time. Using the folding theorem on the time dependence, (2.16) and (2.17) simplify in the space–frequency domain. Thus, for two functions $f = f(t)$ and $g(t)$ the folding theorem

$$[f * g](t) \equiv \int_{-\infty}^{\infty} f(t - t')g(t') dt' = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(\omega)g(\omega)e^{-i\omega t} d\omega \quad (3.9)$$

states that the Fourier transform of $[f * g](t)$ is just the product of the Fourier transforms of $f(t)$ and $g(t)$. In the space–frequency domain, (2.16) and (2.17) hence take the forms

$$\mathbf{A}(\mathbf{r}; \omega) = \mu_0 \int_{-\infty}^{\infty} g(R; \omega) \mathbf{J}(\mathbf{r}'; \omega) d^3 r', \quad (3.10)$$

$$\phi(\mathbf{r}; \omega) = \epsilon_0^{-1} \int_{-\infty}^{\infty} g(R; \omega) \rho(\mathbf{r}'; \omega) d^3 r', \quad (3.11)$$

with $R = |\mathbf{r} - \mathbf{r}'|$, as before. A knowledge of $\mathbf{A}(\mathbf{r}; \omega)$ and $\phi(\mathbf{r}; \omega)$ allows one to obtain the microscopic electric field in the space–frequency domain via

$$\mathbf{E}(\mathbf{r}; \omega) = i\omega \mathbf{A}(\mathbf{r}; \omega) - \nabla \phi(\mathbf{r}; \omega), \quad (3.12)$$

cf. (2.7), and the association in (3.4). An explicit expression is readily obtained for the scalar propagator $g(R; \omega)$. Thus,

$$g(R; \omega) = \int_{-\infty}^{\infty} (4\pi R)^{-1} \delta\left(\frac{R}{c_0} - \tau\right) e^{i\omega\tau} d\tau = \frac{1}{4\pi R} e^{iq_0 R}, \quad (3.13)$$

where

$$q_0 = \frac{\omega}{c_0}. \quad (3.14)$$

The idea behind the dyadic Green function formalism is to express the relation between the electric field, $\mathbf{E}(\mathbf{r}; \omega)$, and the particle dynamics in such a manner that only the current density, $\mathbf{J}(\mathbf{r}; \omega)$, appears on the particle side. The relation between $\mathbf{E}(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$ will be an integral equation, and apart from a constant, the dyadic kernel of this equation will be our Green function for the electric field. The Green function formalism hence presents the implicit solution for the electric field of the Maxwell–Lorentz equations in the space–frequency domain in a very “economic” form. It is perhaps not surprising that such a formalism can be established starting from (3.10)–(3.12) because the equation of continuity in (2.108), which in the space–frequency domain takes the form

$$\nabla \cdot \mathbf{J}(\mathbf{r}; \omega) = i\omega\rho(\mathbf{r}; \omega), \quad (3.15)$$

allows one to eliminate $\rho(\mathbf{r}; \omega)$ in favor of $\mathbf{J}(\mathbf{r}; \omega)$ in (3.11). Upon partial integration one obtains

$$\begin{aligned} \phi(\mathbf{r}; \omega) &= (i\epsilon_0\omega)^{-1} \int_{-\infty}^{\infty} g(R; \omega) \nabla' \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r' \\ &= -(i\epsilon_0\omega)^{-1} \int_{-\infty}^{\infty} \nabla' g(R; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r', \end{aligned} \quad (3.16)$$

since the product $g\mathbf{J}$ vanishes faster than r^{-2} at infinity. Utilizing that $\nabla'g = -\nabla g$, one gets

$$\phi(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \int_{-\infty}^{\infty} \nabla g(R; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r', \quad (3.17)$$

and then

$$\nabla\phi(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \nabla \int_{-\infty}^{\infty} \nabla g(R; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r'. \quad (3.18)$$

In the Green function formalism, one wants to move the ∇ -operator inside the integral in (3.18). If one by brute force interchange the integral and differentiation operations one ends up with a function $\nabla\nabla g$ which exhibits a singularity of the form R^{-3} at $\mathbf{r} = \mathbf{r}'$, since g has a R^{-1} singularity at this point; see (3.13). The integral, thus, is only conditionally convergent. In general one therefore expects

$$\nabla \int_{-\infty}^{\infty} (\dots) d^3r' \neq \int_{-\infty}^{\infty} \nabla(\dots) d^3r'. \quad (3.19)$$

The conclusion in (3.19) turns out to be important for the quantum theory of near-field electrodynamics, and in the theory of spatial photon localization. We shall return to the problem in Chap. 13, and in other passages in the book. In the following we shall be interested in the electric field only at points ($\mathbf{r}$) outside the current density distribution. The Huygens propagator has no singularity in these points, and one can therefore safely interchange the ∇ - and $\int_{-\infty}^{\infty}$ -operations that is

$$\nabla\phi(\mathbf{r};\omega) = (i\epsilon_0\omega)^{-1} \int_{-\infty}^{\infty} \nabla\nabla g(R;\omega) \cdot \mathbf{J}(\mathbf{r}';\omega) d^3r', \quad R \neq 0. \quad (3.20)$$

A combination of (3.10)–(3.12) and (3.20) now readily leads to the following result:

$$\mathbf{E}(\mathbf{r};\omega) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r} - \mathbf{r}';\omega) \cdot \mathbf{J}(\mathbf{r}';\omega) d^3r', \quad (3.21)$$

where, with $\mathbf{r} - \mathbf{r}' = \mathbf{R}$,

$$\mathbf{G}(\mathbf{R};\omega) = (\mathbf{U} + \frac{1}{q_0^2} \nabla\nabla)g(R;\omega), \quad R \neq 0 \quad (3.22)$$

is a dyadic Green function for the electric field [18, 24, 45–48]. If the total current density can be split into source and system parts, $\mathbf{J} = \mathbf{J}_{\text{source}} + \mathbf{J}_{\text{syst}}$, as described in Sect. 2.3., one obtains for field points outside the two current density domains

$$\mathbf{E}(\mathbf{r};\omega) = \mathbf{E}_{\text{source}}(\mathbf{r};\omega) + i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r} - \mathbf{r}';\omega) \cdot \mathbf{J}_{\text{syst}}(\mathbf{r}';\omega) d^3r', \quad (3.23)$$

where the electric field from the source

$$\mathbf{E}_{\text{source}}(\mathbf{r};\omega) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r} - \mathbf{r}';\omega) \cdot \mathbf{J}_{\text{source}}(\mathbf{r}';\omega) d^3r' \quad (3.24)$$

often (but in general not in near-field electrodynamics) may be considered as a prescribed quantity.

3.2.2 Green Function for the Magnetic Field

In the previous subsection, an integral relation between the microscopic electric field and the particle current density was established (3.21), and the kernel (Green function for the electric field) was determined (3.22). We shall show now that an analogous integral relation, viz.,

$$\mathbf{B}(\mathbf{r};\omega) = \frac{i\mu_0\omega}{c_0} \int_{-\infty}^{\infty} \mathbf{G}_M(\mathbf{r} - \mathbf{r}';\omega) \cdot \mathbf{J}(\mathbf{r}';\omega) d^3r', \quad (3.25)$$

can be established between the microscopic magnetic field and the current density, and we shall find an explicit expression for the Green function of the magnetic (M) field, $\mathbf{G}_M(\mathbf{R}; \omega)$, in the space–frequency domain. The factors in front of the integrals in (3.21) and (3.25) deviate by a factor c_0^{-1} , and this implies that the two Green functions $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_M(\mathbf{R}; \omega)$ attain the same dimensionality. As for the electric field case, we shall also here only be interested in the magnetic field outside the current density domain. From the Maxwell–Lorentz equation in (3.5) and (3.21) one readily obtains

$$\mathbf{B}(\mathbf{r}; \omega) = \mu_0 \int_{-\infty}^{\infty} \nabla \times [\mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega)] d^3 r', \quad (3.26)$$

since the curl and integral operations can be interchanged, cf. the discussion above the inequality in (3.19).

By means of the tensor relation

$$\nabla \times (\mathbf{A} \mathbf{B}) = (\nabla \times \mathbf{A}) \mathbf{B} - (\mathbf{A} \times \nabla) \mathbf{B} \quad (3.27)$$

one gets $\nabla \times [\mathbf{A} \mathbf{B} \cdot \mathbf{C}] = (\nabla \times \mathbf{A})(\mathbf{B} \cdot \mathbf{C}) - \mathbf{A} \times \nabla(\mathbf{B} \cdot \mathbf{C}) = [\nabla \times (\mathbf{A} \mathbf{B})] \cdot \mathbf{C}$, and since $\mathbf{G}(\mathbf{R}; \omega)$ is a sum of tensor products one has $\nabla \times (\mathbf{G} \cdot \mathbf{J}) = (\nabla \times \mathbf{G}) \cdot \mathbf{J}$. With this result inserted in (3.26), a comparison to (3.25) shows that the dyadic Green functions for the electric and magnetic fields are related as follows:

$$\mathbf{G}_M(\mathbf{R}; \omega) = (i q_0)^{-1} \nabla \times \mathbf{G}(\mathbf{R}; \omega). \quad (3.28)$$

By insertion of (3.22) into (3.28), and use of the fact

$$\nabla \times \nabla \nabla g(R; \omega) = \hat{\mathbf{R}} \times \hat{\mathbf{R}} \hat{\mathbf{R}} \frac{\partial^3}{\partial R^3} g(R; \omega) = \mathbf{0}, \quad (3.29)$$

it appears that

$$\mathbf{G}_M(\mathbf{R}; \omega) = (i q_0)^{-1} \nabla \times (\mathbf{U} g(R; \omega)), \quad (3.30)$$

and then finally

$$\mathbf{G}_M(\mathbf{R}; \omega) = (i q_0)^{-1} \mathbf{U} \times \nabla g(R; \omega). \quad (3.31)$$

Since the right side of (3.31) is the cross product of the unit tensor, $\mathbf{U} = \hat{\mathbf{x}} \hat{\mathbf{x}} + \hat{\mathbf{y}} \hat{\mathbf{y}} + \hat{\mathbf{z}} \hat{\mathbf{z}}$, with some vector, $(i q_0)^{-1} \nabla g$, the Green function for the magnetic field is an antisymmetric tensor, as one might have expected.

3.3 Near-, Mid-, and Far-Field Parts of $\mathbf{G}$ and $\mathbf{G}_M$

3.3.1 Green Functions in Spherical Coordinates

In near-field electrodynamics as such, and for many other purposes, e.g., in studies of emission and scattering of electromagnetic fields from point particles (electrons,

muons, ...), atoms, and mesoscopic objects, it is of interest to express the Green functions for the electric and magnetic fields in spherical coordinates centered on $\mathbf{R} = \mathbf{0}$. Closed-form expressions are obtained for $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_M(\mathbf{R}; \omega)$ in these coordinates. Since the Huygens propagator only depends on the magnitude of $\mathbf{R}$, only the radial part, $\hat{\mathbf{R}} \partial/\partial R$, of ∇ is needed for the calculation. The results one obtains are the following:

$$\mathbf{G}(\mathbf{R}; \omega) = \frac{iq_0}{4\pi} \left\{ \frac{1}{iq_0 R} (U - \hat{\mathbf{R}} \hat{\mathbf{R}}) - \left[\frac{1}{(iq_0 R)^2} - \frac{1}{(iq_0 R)^3} \right] (U - 3\hat{\mathbf{R}} \hat{\mathbf{R}}) \right\} e^{iq_0 R}, \quad (3.32)$$

and

$$\mathbf{G}_M(\mathbf{R}; \omega) = \frac{iq_0}{4\pi} \left[\frac{1}{iq_0 R} - \frac{1}{(iq_0 R)^2} \right] e^{iq_0 R} \mathbf{U} \times \hat{\mathbf{R}}, \quad (3.33)$$

where

$$U = \hat{\mathbf{R}} \hat{\mathbf{R}} + \hat{\boldsymbol{\Theta}} \hat{\boldsymbol{\Theta}} + \hat{\boldsymbol{\Phi}} \hat{\boldsymbol{\Phi}} \quad (3.34)$$

is the unit tensor expressed in terms of the usual local unit vector $\hat{\mathbf{R}}$ (radial), $\hat{\boldsymbol{\Theta}}$ (polar), and $\hat{\boldsymbol{\Phi}}$ (azimuthal) of the spherical coordinate system. Since $\hat{\boldsymbol{\Theta}} \times \hat{\mathbf{R}} = -\hat{\boldsymbol{\Phi}}$ and $\hat{\boldsymbol{\Phi}} \times \hat{\mathbf{R}} = \hat{\boldsymbol{\Theta}}$, the Green function for the magnetic field can also be written in the form

$$\mathbf{G}_M(\mathbf{R}; \omega) = \frac{iq_0}{4\pi} \left[\frac{1}{iq_0 R} - \frac{1}{(iq_0 R)^2} \right] e^{iq_0 R} (\hat{\boldsymbol{\Phi}} \hat{\boldsymbol{\Theta}} - \hat{\boldsymbol{\Theta}} \hat{\boldsymbol{\Phi}}). \quad (3.35)$$

The antisymmetric form of $\mathbf{G}_M(\mathbf{R}; \omega)$ is manifest in (3.35). The magnitude of the electromagnetic field which is generated in the observation point $\mathbf{r}$ by the current density $\mathbf{J}(\mathbf{r}'; \omega)$ in the infinitesimal volume d^3r' located at $\mathbf{r}'$ depends strongly on the numerical distance between these points. Quantitatively, it is the distance measured in electromagnetic wavelengths divided by 2π , i.e., $q_0 R$, which is the important quantity. It appears from (3.32) that $\mathbf{G}(\mathbf{R}; \omega)$, apart from an overall oscillating factor $\exp(iq_0 R)$, consists of a sum of dyadic terms having the distance dependences $(q_0 R)^{-1}$, $(q_0 R)^{-2}$, and $(q_0 R)^{-3}$. For $\mathbf{G}_M(\mathbf{R}; \omega)$ there is no $(q_0 R)^{-3}$ dependence.

3.3.2 Far-Field Zone

If the source and observation points are sufficiently far from each other ($q_0 R \gg 1$), the terms proportional to $(q_0 R)^{-1}$ will in general be the dominating ones in $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_M(\mathbf{R}; \omega)$. The far-field parts (superscript FF) of the two Green functions are

$$\mathbf{G}^{\text{FF}}(\mathbf{R}; \omega) = \frac{e^{iq_0 R}}{4\pi R} (U - \hat{\mathbf{R}} \hat{\mathbf{R}}), \quad (3.36)$$

and

$$\mathbf{G}_M^{\text{FF}}(\mathbf{R}; \omega) = \frac{e^{iq_0 R}}{4\pi R} \left(\hat{\boldsymbol{\Phi}} \hat{\boldsymbol{\Theta}} - \hat{\boldsymbol{\Theta}} \hat{\boldsymbol{\Phi}} \right). \quad (3.37)$$

The scalar factor $\exp(iq_0 R)/(4\pi R)$ is the same for the two far-field Green functions, and just the Huygens propagator (3.13). The dyadic factors $\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}$ and $\hat{\boldsymbol{\Phi}}\hat{\boldsymbol{\Theta}} - \hat{\boldsymbol{\Theta}}\hat{\boldsymbol{\Phi}}$ show that the electric and magnetic far fields in the observation point both lie in a plane perpendicular to the direction from the source (at $\mathbf{r}'$) to the observation point. This in turn tells us that there is no electromagnetic far field in observation points located along the current density direction, i.e., for $\mathbf{R} \parallel \mathbf{J}(\mathbf{r}'; \omega) d^3 r'$. The far-field zone is also called the (purely) radiative zone. From a fundamental point of view only transverse photons are responsible for the energy, momentum, and angular momentum flow away from the source point in the far field as we shall realize later on. Since the common scalar factor in (3.36) and (3.37) is the Huygens propagator the far-field Green functions also exist in the space–time domain, cf. (2.18) and (3.13). The existence of the far-field Green functions $\mathbf{G}^{\text{FF}}(\mathbf{R}; \omega)$ and $\mathbf{G}_M^{\text{FF}}(\mathbf{R}; \omega)$ is a necessity also because transverse photons always propagate with the vacuum speed of light.

3.3.3 Mid-Field Terms

In the intermediate zone, i.e., for $q_0 R \sim 1$, the terms proportional to $(q_0 R)^{-2}$ make a substantial contribution to the Green functions for the electric and magnetic fields. The explicit expressions for these so-called mid-field (MF) terms are

$$\mathbf{G}^{\text{MF}}(\mathbf{R}; \omega) = \frac{e^{iq_0 R}}{4\pi R} \frac{1}{iq_0 R} \left(3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U} \right), \quad (3.38)$$

$$\mathbf{G}_M^{\text{MF}}(\mathbf{R}; \omega) = \frac{e^{iq_0 R}}{4\pi R} \frac{1}{iq_0 R} \left(\hat{\boldsymbol{\Theta}}\hat{\boldsymbol{\Phi}} - \hat{\boldsymbol{\Phi}}\hat{\boldsymbol{\Theta}} \right). \quad (3.39)$$

The tensorial form of $\mathbf{G}_M^{\text{MF}}(\mathbf{R}; \omega)$ shows that the magnetic field from the source $\mathbf{J}(\mathbf{r}'; \omega) d^3 r'$ is perpendicular to the $\hat{\mathbf{R}}$ -direction. This is not the case for $\mathbf{G}^{\text{MF}}(\mathbf{R}; \omega)$, however. Since $\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} = \hat{\boldsymbol{\Theta}}\hat{\boldsymbol{\Theta}} + \hat{\boldsymbol{\Phi}}\hat{\boldsymbol{\Phi}} - 2\hat{\mathbf{R}}\hat{\mathbf{R}}$, the electric field from $\mathbf{J}(\mathbf{r}'; \omega) d^3 r'$ also has a component along the $\hat{\mathbf{R}}$ -direction in general. The magnetic mid field vanishes for observation points in the $\hat{\mathbf{R}}$ -direction, and since, as discussed in Sect. 3.3.2, also the entire far field vanishes in this direction, the dominating part of the electromagnetic field in the $\hat{\mathbf{R}}$ -direction at large distance is a magnetic mid-field term.

3.3.4 Near-Field Zone

The Green function for the magnetic field has no near-field $((q_0 R)^{-3})$ part, and when $q_0 R \ll 1$ it is often sufficient to replace the full Green function for the electric

field by its near-field (NF) part

$$\mathbf{G}^{\text{NF}}(\mathbf{R}; \omega) = \frac{e^{iq_0 R}}{4\pi R} \frac{1}{(iq_0 R)^2} \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} \right). \quad (3.40)$$

In near-field optics, where electrodynamic interactions over distances satisfying the inequality $q_0 R \ll 1$ often are studied, it is in many cases sufficient to replace the full Green function for the electric field by $\mathbf{G}^{\text{NF}}(\mathbf{R}; \omega)$. The near-field Green function may be characterized as a quasi-static Green function, and if the small distance dependent phase shift contained in the $\exp(iq_0 R)$ factor can be neglected one has

$$\mathbf{G}^{\text{NF}}(\mathbf{R}; \omega) = \frac{3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U}}{4\pi q_0^2 R^3}. \quad (3.41)$$

In near-field interactions based on (3.41) retardation effects are neglected, as we shall realize when we discuss near-field electrodynamics in the space–time domain later on.

3.4 Green Functions and Wave Equations in the Space–Frequency Domain

It is well known that the Huygens propagator in (3.13) satisfies the singular differential equation

$$(\nabla^2 + q_0^2)g(R; \omega) = -\delta(\mathbf{r} - \mathbf{r}'), \quad (3.42)$$

and from (2.14) and the association in (3.4), it follows that the vector potential in the Lorenz gauge satisfies the inhomogeneous wave equation

$$(\nabla^2 + q_0^2)\mathbf{A}(\mathbf{r}; \omega) = -\mu_0 \mathbf{J}(\mathbf{r}; \omega). \quad (3.43)$$

Multiplying (3.42) with $\mathbf{J}(\mathbf{r}'; \omega)$, and integrating thereafter the resulting equation over $\mathbf{r}'$ -space, one obtains

$$\int_{-\infty}^{\infty} (\nabla^2 + q_0^2)g(R; \omega) \mathbf{J}(\mathbf{r}'; \omega) d^3 r' = -\mathbf{J}(\mathbf{r}; \omega). \quad (3.44)$$

For observation points outside the current density domain the operations $\int_{-\infty}^{\infty}$ and $\nabla^2 + q_0^2$ can be interchanged. Doing this (3.44) takes the same form as (3.43). In turn it follows that the particular (physical) solution for the vector potential is related to the current density by the integral form in (3.4).

Let us now consider the linear dyadic differential operator

$$\mathcal{L}(\nabla; \omega) = \mathbf{U}(\nabla^2 + q_0^2) - \nabla \nabla, \quad (3.45)$$

which deviates from the dyadic Helmholtz operator $U(\nabla^2 + q_0^2)$ by a term $\nabla\nabla$. Letting $\mathcal{L}$ operate on the dyadic Green function for the electric field (3.22) one readily gets

$$\mathcal{L}(\nabla; \omega) \cdot \mathbf{G}(\mathbf{R}; \omega) = -\delta(\mathbf{r} - \mathbf{r}')U. \quad (3.46)$$

There are certain difficulties related to the general solution of an equation of the form given in (3.46). We shall study these in Chap. 14, but the reader may perhaps already have realized the problem due to the fact that the formula for $\mathbf{G}(\mathbf{R}; \omega)$ given in (3.22) necessitates that $R \neq 0$. The Helmholtz operator $\nabla^2 + q_0^2$ acting on the Huygens propagator gives a delta function at $\mathbf{r} - \mathbf{r}'$ (multiplied by -1). In analogy to this, the operator $\mathcal{L}(\nabla; \omega)$ when acting on the Green function for the electric field equals a delta function located at $\mathbf{r} - \mathbf{r}'$ (multiplied by $-U$). By taking the curl of (3.5) and replacing then $\nabla \times \mathbf{B}$ by the right side of (3.7) it appears that the microscopic Maxwell–Lorentz equations result in the following inhomogeneous wave equation for the electric field:

$$\nabla \times (\nabla \times \mathbf{E}(\mathbf{r}; \omega)) - q_0^2 \mathbf{E}(\mathbf{r}; \omega) = i\mu_0\omega \mathbf{J}(\mathbf{r}; \omega), \quad (3.47)$$

or equivalently

$$\mathcal{L}(\nabla; \omega) \cdot \mathbf{E}(\mathbf{r}; \omega) = -i\mu_0\omega \mathbf{J}(\mathbf{r}; \omega). \quad (3.48)$$

Scalar multiplication of (3.40) with $\mathbf{J}(\mathbf{r}'; \omega)$ from the right, integration over the $\mathbf{r}'$ -domain, and interchange of the operations $\int_{-\infty}^{\infty}$ and $\mathcal{L}$ lead upon comparison to (3.48) to the conclusion that the microscopic electric field and the current density are related via the integral relation given in (3.21), provided the point of observation is located outside the current density domain.

A combination of the microscopic Maxwell–Lorentz equations in (3.5) and (3.7) shows that the magnetic field satisfies the inhomogeneous wave equation

$$\nabla \times (\nabla \times \mathbf{B}(\mathbf{r}; \omega)) - q_0^2 \mathbf{B}(\mathbf{r}; \omega) = \mu_0 \nabla \times \mathbf{J}(\mathbf{r}; \omega), \quad (3.49)$$

which by means of (3.8) can be simplified to

$$(\nabla^2 + q_0^2) \mathbf{B}(\mathbf{r}; \omega) = -\mu_0 \nabla \times \mathbf{J}(\mathbf{r}; \omega). \quad (3.50)$$

The relevant differential operator for the wave equation for the electric field (3.48) is $\mathcal{L}(\nabla; \omega)$ (3.45). For the wave equation for the magnetic field it is the simpler scalar Helmholtz operator $\nabla^2 + q_0^2$, because $\nabla \cdot \mathbf{B}(\mathbf{r}; \omega) = 0$. To establish the singular differential equation for the Green function for the magnetic field, $\mathbf{G}_M(\mathbf{R}; \omega)$, we let the Helmholtz operator work on (3.31). Thus, using (3.42) we obtain

$$\begin{aligned} (\nabla^2 + q_0^2) \mathbf{G}_M(\mathbf{R}; \omega) &= (iq_0)^{-1} U \times \nabla (\nabla^2 + q_0^2) g(\mathbf{R}; \omega) \\ &= -(iq_0)^{-1} U \times \nabla \delta(\mathbf{r} - \mathbf{r}'), \end{aligned} \quad (3.51)$$

and $\mathbf{G}_M(\mathbf{R}; \omega)$ multiplied by $i q_0$ therefore satisfies the singular differential equation

$$(\nabla^2 + q_0^2)(i q_0 \mathbf{G}_M(\mathbf{R}; \omega)) = -\mathbf{U} \times \nabla \delta(\mathbf{r} - \mathbf{r}'). \quad (3.52)$$

The singular matrix on the right side of (3.46) is antisymmetric, i.e.,

$$-\mathbf{U} \times \nabla \delta = \begin{pmatrix} 0 & \frac{\partial \delta}{\partial z} & -\frac{\partial \delta}{\partial y} \\ -\frac{\partial \delta}{\partial z} & 0 & \frac{\partial \delta}{\partial x} \\ \frac{\partial \delta}{\partial y} & -\frac{\partial \delta}{\partial x} & 0 \end{pmatrix}, \quad (3.53)$$

as it must be because $\mathbf{G}_M(\mathbf{R}; \omega)$ is an antisymmetric tensor. The matrix depends on the gradient of the delta function, and this can be traced back to the fact that $\nabla \times \mathbf{J}(\mathbf{r}; \omega)$ occurs in the wave equation for the magnetic field (3.50), and $\mathbf{J}(\mathbf{r}; \omega)$ in the integral expression for $\mathbf{B}(\mathbf{r}; \omega)$ (3.25). Together, (3.50) and (3.52) lead back to the integral relation between $\mathbf{B}(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$ given in (3.25). To realize this let us take the scalar product of (3.52) with $\mathbf{J}(\mathbf{r}', \omega)$ from the right and then integrate over $\mathbf{r}'$ -space. Hence,

$$i q_0 \int_{-\infty}^{\infty} (\nabla^2 + q_0^2) \mathbf{G}_M(\mathbf{R}; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r' = - \int_{-\infty}^{\infty} \mathbf{U} \times \nabla \delta(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r'. \quad (3.54)$$

Interchange of the $\int_{-\infty}^{\infty}$ - and $\nabla^2 + q_0^2$ - operations on the left side of this equation, and use of $\nabla \delta(\mathbf{r} - \mathbf{r}') = -\nabla' \delta(\mathbf{r} - \mathbf{r}')$ followed by a partial integration on the right side of the equation give

$$i q_0 (\nabla^2 + q_0^2) \int_{-\infty}^{\infty} \mathbf{G}_M(\mathbf{R}; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r' = -\nabla \times \mathbf{J}(\mathbf{r}; \omega). \quad (3.55)$$

A comparison of (3.50) and (3.55) finally gives (3.25).

3.5 Spectral Representation of the Electromagnetic Field from an Assembly of Moving Point Particles

In the space–frequency domain the current density of an assembly of point particles is given by

$$\mathbf{J}(\mathbf{r}; \omega) = \sum_{\alpha} q_{\alpha} \int_{-\infty}^{\infty} \mathbf{v}_{\alpha}(t) \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) e^{i \omega t} dt \quad (3.56)$$

in the notation used in (2.29). If (3.56) is inserted into (3.21), and the integrations over $\mathbf{r}'$ -space and time (t') are interchanged, one obtains for the electric field the result

$$\mathbf{E}(\mathbf{r}; \omega) = i\mu_0\omega \sum_{\alpha} q_{\alpha} \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{r} - \mathbf{r}_{\alpha}(t); \omega) \cdot \mathbf{v}_{\alpha}(t) e^{i\omega t} dt, \quad (3.57)$$

since the presence of the delta functions, $\delta(\mathbf{r}' - \mathbf{r}_{\alpha}(t))$, readily allows one to carry out the $\mathbf{r}'$ -integrations. In analogy to (3.57), the magnetic field is given by

$$\mathbf{B}(\mathbf{r}; \omega) = \frac{i\mu_0\omega}{c_0} \sum_{\alpha} \int_{-\infty}^{\infty} \mathbf{G}_M(\mathbf{r} - \mathbf{r}_{\alpha}(t); \omega) \cdot \mathbf{v}_{\alpha}(t) e^{i\omega t} dt. \quad (3.58)$$

The spectral representations in (3.57) and (3.58) are useful for studies of e.g., (1) multipole radiation from a well localized distribution of slowly moving charges, (2) Cherenkov [44, 45] and Cherenkov–Landau [5, 161, 162] shock waves, (3) electric dipole-surface interaction, and (4) energy, momentum, and angular-momentum calculations of the electromagnetic field emitted from an oscillating point-particle.

Chapter 4

Angular Spectrum Representation of the Green Functions and Fields

4.1 Maxwell–Lorentz Equations in Mixed Representation

In Sect. 3.1, we made a Fourier integral analysis of the time dependence of the Maxwell–Lorentz equations. Now we go one step further and make also a partial Fourier transformation of the space dependent part of these equations. For a vector field $\mathbf{V}(\mathbf{r}; \omega)$ described in Cartesian coordinates (x, y, z) we thus carry out Fourier integral transformations on the x - and y -dependences. Thus,

$$\mathbf{V}(z; \mathbf{q}_{\parallel}, \omega) = \int_{-\infty}^{\infty} \mathbf{V}(\mathbf{r}; \omega) e^{-i\mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel}} d^2 r_{\parallel}, \quad (4.1)$$

where $\mathbf{r}_{\parallel} = (x, y, 0)$, $\mathbf{q}_{\parallel} = (q_x, q_y, 0)$ and $d^2 r = dx dy$. From a physical point of view we have hence made a plane-wave decomposition of the vector field perpendicular to the z -axis. The two-dimensional wave vector is denoted by $\mathbf{q}_{\parallel}$. The direction of the z -axis is of course arbitrary. The inverse transformation to (4.1) is

$$\mathbf{V}(\mathbf{r}; \omega) = (2\pi)^{-2} \int_{-\infty}^{\infty} \mathbf{V}(z; \mathbf{q}_{\parallel}, \omega) e^{i\mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel}} d^2 q_{\parallel}, \quad (4.2)$$

where $d^2 q_{\parallel} = dq_x dq_y$. With the sign convention on the arguments of the exponentials in (4.1) and (4.2), plane-wave propagation perpendicular to the z -axis is described in the usual form $\sim \exp[i(\mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel} - \omega t)]$. By combining (3.3) and (4.2) one gets the following decomposition of the vector field $\mathbf{V}(\mathbf{r}, t)$ in monochromatic, two-dimensional plane-wave components:

$$\mathbf{V}(\mathbf{r}, t) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{V}(z; \mathbf{q}_{\parallel}, \omega) e^{i(\mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel} - \omega t)} d^2 q_{\parallel} d\omega. \quad (4.3)$$

The decomposition in (4.3) of the arbitrary space–time vector field $\mathbf{V}(\mathbf{r}, t)$ is called the angular spectrum representation. In this decomposition the arbitrary space–time vector field $\mathbf{V}(\mathbf{r}, t)$ is represented by the transformed quantity $\mathbf{V}(z; \mathbf{q}_{\parallel}, \omega)$. Since the transforms of $\nabla \times \mathbf{V}(\mathbf{r}, t)$ and $\nabla \cdot \mathbf{V}(\mathbf{r}, t)$ are $\mathcal{O} \times \mathbf{V}(z; \mathbf{q}_{\parallel}, \omega)$ and $\mathcal{O} \cdot \mathbf{V}(z; \mathbf{q}_{\parallel}, \omega)$,

where

$$\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) = i\mathbf{q}_{\parallel} + \hat{\mathbf{z}}\frac{\partial}{\partial z}, \quad (4.4)$$

the prescription

$$\nabla \Leftrightarrow i\mathbf{q}_{\parallel} + \hat{\mathbf{z}}\frac{\partial}{\partial z} \quad (4.5)$$

readily allows one to write down the Maxwell–Lorentz equations among the angular spectrum representatives of the vector and scalar fields, $\mathbf{E}$, $\mathbf{B}$, $\mathbf{J}$ and ρ . Thus, from (3.5)–(3.8) we obtain the following electrodynamic equations:

$$\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \times \mathbf{E}(z; \mathbf{q}_{\parallel}, \omega) = i\omega \mathbf{B}(z; \mathbf{q}_{\parallel}, \omega), \quad (4.6)$$

$$\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \cdot \mathbf{E}(z; \mathbf{q}_{\parallel}, \omega) = \frac{1}{\epsilon_0} \rho(z; \mathbf{q}_{\parallel}, \omega), \quad (4.7)$$

$$\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \times \mathbf{B}(z; \mathbf{q}_{\parallel}, \omega) = \mu_0 \mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) - \frac{i\omega}{c_0^2} \mathbf{E}(z; \mathbf{q}_{\parallel}, \omega) \quad (4.8)$$

$$\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \cdot \mathbf{B}(z; \mathbf{q}_{\parallel}, \omega) = 0. \quad (4.9)$$

With the prescription in (4.5) it appears that the dyadic differential operator $\mathcal{L}(\nabla; \omega)$ in (3.45) takes the form

$$\begin{aligned} & \mathcal{L}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}, \omega\right) \\ &= \left[\mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \cdot \mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) + q_0^2 \right] U - \mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \mathcal{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel}\right) \end{aligned} \quad (4.10)$$

in the mixed representation, and the inhomogeneous wave equation for the electric field $\mathbf{E}(z; \mathbf{q}_{\parallel}, \omega)$, therefore, is given by

$$\begin{aligned} & \left[U \left(q_0^2 - q_{\parallel}^2 + \frac{\partial^2}{\partial z^2} \right) + \mathbf{q}_{\parallel} \mathbf{q}_{\parallel} - \hat{\mathbf{z}} \hat{\mathbf{z}} \frac{\partial^2}{\partial z^2} - i \left(\mathbf{q}_{\parallel} \hat{\mathbf{z}} + \hat{\mathbf{z}} \mathbf{q}_{\parallel} \right) \frac{\partial}{\partial z} \right] \cdot \mathbf{E}(z; \mathbf{q}_{\parallel}, \omega) \\ &= -i\mu_0 \omega \mathbf{J}(z; \mathbf{q}_{\parallel}, \omega). \end{aligned} \quad (4.11)$$

The corresponding inhomogeneous wave equation for the magnetic field $\mathbf{B}(z; \mathbf{q}_{\parallel}, \omega)$ becomes

$$\left(q_0^2 - q_{\parallel}^2 + \frac{\partial^2}{\partial z^2} \right) \mathbf{B}(z; \mathbf{q}_{\parallel}, \omega) = -\mu_0 \left(i\mathbf{q}_{\parallel} + \hat{\mathbf{z}} \frac{\partial}{\partial z} \right) \times \mathbf{J}(z; \mathbf{q}_{\parallel}, \omega), \quad (4.12)$$

as one immediately realizes from (3.50) and the prescription in (4.5).

4.2 Interlude: Monochromatic Plane-Wave Representation of the Maxwell–Lorentz Equations and Green Functions

If the various vector and scalar fields in the Maxwell–Lorentz equations in (2.1)–(2.4) are Fourier integral analyzed fully in both space and time according to the transformation

$$V(\mathbf{r}, t) = (2\pi)^{-4} \int_{-\infty}^{\infty} V(\mathbf{q}, \omega) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} d^3q d\omega, \quad (4.13)$$

where the Fourier amplitude $V(\mathbf{q}, \omega)$ is given by the inverse transformation

$$V(\mathbf{q}, \omega) = \int_{-\infty}^{\infty} V(\mathbf{r}, t) e^{-i(\mathbf{q} \cdot \mathbf{r} - \omega t)} d^3r dt, \quad (4.14)$$

the electrodynamic equations become algebraic equations among the various Fourier amplitudes. These algebraic equations are easily obtained from (3.5)–(3.8) using the prescription

$$\nabla \Leftrightarrow i\mathbf{q}. \quad (4.15)$$

Hence,

$$\mathbf{q} \times \mathbf{E}(\mathbf{q}, \omega) = \omega \mathbf{B}(\mathbf{q}, \omega), \quad (4.16)$$

$$i\mathbf{q} \cdot \mathbf{E}(\mathbf{q}, \omega) = \frac{1}{\epsilon_0} \rho(\mathbf{q}, \omega), \quad (4.17)$$

$$i\mathbf{q} \times \mathbf{B}(\mathbf{q}, \omega) = \mu_0 \mathbf{J}(\mathbf{q}, \omega) - \frac{i\omega}{c_0^2} \mathbf{E}(\mathbf{q}, \omega), \quad (4.18)$$

$$\mathbf{q} \cdot \mathbf{B}(\mathbf{q}, \omega) = 0. \quad (4.19)$$

The algebraic form of the set of microscopic Maxwell–Lorentz equations is of great interest in its own right, and in the following subsection this form will be used in connection with the derivation of the angular spectrum representations of the scalar Huygens propagator and the dyadic Green functions for the electric and magnetic fields.

If one makes a Fourier integral analysis of the z -dependence of $V(z; \mathbf{q}_{\parallel}, \omega)$, i.e.,

$$V(z; \mathbf{q}_{\parallel}, \omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} V(q_{\perp}, \mathbf{q}_{\parallel}, \omega) e^{iq_{\perp}z} dq_{\perp}, \quad (4.20)$$

where $q_{\perp}$ is the relevant Fourier variable, it appears that the wave vectors $\mathbf{q}_{\parallel}$ and $\mathbf{q}$ are related via

$$\mathbf{q} = \mathbf{q}_{\parallel} + q_{\perp} \hat{\mathbf{z}}. \quad (4.21)$$

In general, the quantity $q_{\perp} \hat{\mathbf{z}}$ thus is the component of the total wave vector $\mathbf{q}$ in the direction perpendicular ($\perp$) to the planes over which the vector field was Fourier integral transformed in the mixed representation.

The plane-wave representation of the scalar propagator $g(R; \omega)$ can be obtained inserting the Fourier integral transformations

$$g(R; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} g(q, \omega) e^{i\mathbf{q} \cdot \mathbf{R}} d^3q, \quad (4.22)$$

and

$$\delta(\mathbf{R}) = (2\pi)^{-3} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{R}} d^3q \quad (4.23)$$

into (3.42). This gives after interchange of the $\nabla^2 + q_0^2$ - and $\int_{-\infty}^{\infty}$ -operations, and differentiation

$$(2\pi)^{-3} \int_{-\infty}^{\infty} [(q_0^2 - q^2)g(q, \omega) + 1] e^{i\mathbf{q} \cdot \mathbf{R}} d^3q = 0. \quad (4.24)$$

Since the integral must vanish for all $\mathbf{R}$'s, one obtains

$$g(q, \omega) = \frac{1}{q^2 - q_0^2}. \quad (4.25)$$

The Huygens propagator in (4.25) is singular for $q = q_0$, and this reflects the fact that $g(R; \omega) = \exp(iq_0 R)/(4\pi R)$ is singular for $R = 0$. Special precautions must therefore be taken when the expression for $g(q, \omega)$ is inserted in (4.22), and the integration over $\mathbf{q}$ -space is carried out; see Sect. 4.3. The isotropy of $g(R; \omega)$ in $\mathbf{R}$ -space implies that the Huygens propagator in wave-vector space can depend only on the magnitude of $\mathbf{q}$, a fact already used in the notation in (4.22).

The plane-wave representation of the dyadic Green function for the electric field can be obtained inserting the expansion in (4.22) into (3.22), or by insertion of the Fourier integral transformation

$$\mathbf{G}(\mathbf{R}; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{G}(\mathbf{q}, \omega) e^{i\mathbf{q} \cdot \mathbf{R}} d^3q \quad (4.26)$$

into (3.46). The last procedure leads to the algebraic equation

$$[\mathbf{U}(q_0^2 - q^2) + \mathbf{q}\mathbf{q}] \cdot \mathbf{G}(\mathbf{q}, \omega) = -\mathbf{U} \quad (4.27)$$

for $\mathbf{G}(\mathbf{q}, \omega)$, and in turn

$$\mathbf{G}(\mathbf{q}, \omega) = \frac{\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}}{q^2 - q_0^2} - \frac{\hat{\mathbf{q}}\hat{\mathbf{q}}}{q_0^2}. \quad (4.28)$$

where $\hat{\mathbf{q}} = \mathbf{q}/q$. The two terms in (4.28) have their own importance, physically. To realize this, let us apply the folding theorem [(3.9)] to (3.21). This gives

$$\mathbf{E}(\mathbf{q}, \omega) = i\mu_0\omega \mathbf{G}(\mathbf{q}, \omega) \cdot \mathbf{J}(\mathbf{q}, \omega). \quad (4.29)$$

The last term in (4.28) thus is seen to relate the components of the electric field ($\hat{\mathbf{q}} \cdot \mathbf{E}(\mathbf{q}, \omega)$) and the current density ($\hat{\mathbf{q}} \cdot \mathbf{J}(\mathbf{q}, \omega)$) along the $\mathbf{q}$ -direction, and the first term of the Green function relates the components of $\mathbf{E}(\mathbf{q}, \omega)$ and $\mathbf{J}(\mathbf{q}, \omega)$ perpendicular to $\hat{\mathbf{q}}$ to each other. There is no cross-coupling between the electric field and current density parallel and perpendicular to the $\mathbf{q}$ -direction, an expected result due to the fact that $\mathbf{G}(\mathbf{q}, \omega)$ relates to plane-wave modes in the isotropic vacuum. The Green function for the electric field may also be written in the alternative form

$$\mathbf{G}(\mathbf{q}, \omega) = \frac{1}{q^2 - q_0^2} \left(\mathbf{U} - \frac{\mathbf{q}\mathbf{q}}{q_0^2} \right), \quad (4.30)$$

which sometimes is useful. Like the Huygens propagator, the dyadic Green function is also singular for $q = q_0$.

The plane-wave representation of the dyadic Green function for the magnetic field is obtained by inserting the Fourier integral transformation

$$\mathbf{G}_M(\mathbf{R}; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{G}_M(\mathbf{q}, \omega) e^{i\mathbf{q} \cdot \mathbf{R}} d^3q \quad (4.31)$$

into (3.52). Calculations analogous to those carried out to determine $\mathbf{G}(\mathbf{R}; \omega)$ result in

$$\mathbf{G}_M(\mathbf{q}, \omega) = \frac{q}{q_0} \frac{1}{q^2 - q_0^2} \mathbf{U} \times \hat{\mathbf{q}}, \quad (4.32)$$

an expression which also is singular for $q = q_0$. The folding theorem in $\mathbf{r}$ -space gives when applied to (3.25)

$$\mathbf{B}(\mathbf{q}, \omega) = \frac{i\mu_0\omega}{c_0} \mathbf{G}_M(\mathbf{q}, \omega) \cdot \mathbf{J}(\mathbf{q}, \omega). \quad (4.33)$$

A current density parallel to the $\mathbf{q}$ -direction does not give rise to a magnetic field, and the magnetic field generated by a current density perpendicular to $\hat{\mathbf{q}}$ always lies in a plane perpendicular to $\hat{\mathbf{q}}$. To prove the above-mentioned claims we expand the unit dyad after a triple set of orthogonal unit vectors $\hat{\mathbf{q}}_{\perp}^{(1)}$, $\hat{\mathbf{q}}_{\perp}^{(2)}$, and $\hat{\mathbf{q}}$, with $\hat{\mathbf{q}}_1^{(1)} \times \hat{\mathbf{q}}_2^{(2)} = \hat{\mathbf{q}}$, i.e.,

$$\mathbf{U} = \hat{\mathbf{q}}_{\perp}^{(1)} \hat{\mathbf{q}}_{\perp}^{(1)} + \hat{\mathbf{q}}_{\perp}^{(2)} \hat{\mathbf{q}}_{\perp}^{(2)} + \hat{\mathbf{q}} \hat{\mathbf{q}}, \quad (4.34)$$

and by inserting this expression for $\mathbf{U}$ into (4.32) we obtain

$$\mathbf{G}_M(\mathbf{q}, \omega) = \frac{q}{q_0} \frac{1}{q^2 - q_0^2} \left(\hat{\mathbf{q}}_{\perp}^{(2)} \hat{\mathbf{q}}_{\perp}^{(1)} - \hat{\mathbf{q}}_{\perp}^{(1)} \hat{\mathbf{q}}_{\perp}^{(2)} \right). \quad (4.35)$$

The truth of the above-mentioned claims follows from (4.33) and (4.35).

4.3 Green Functions in Mixed Representation

4.3.1 Scalar Propagator, $g(Z; q_{\parallel}, \omega)$

It appears from (4.20) (yet, with the vector V replaced by a scalar V), (4.21), and (4.25) that the Huygens propagator in the mixed representation is given by the integral

$$g(Z; q_{\parallel}, \omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} \frac{e^{iq_{\perp}Z} dq_{\perp}}{q_{\perp}^2 + q_{\parallel}^2 - q_0^2}. \quad (4.36)$$

Remembering that $q_{\parallel}$ can attain arbitrary values in the entire range $0 \leq q_{\parallel} < \infty$, cf. (4.2), it turns out to be useful to introduce the quantity $\kappa_{\perp}$ as follows:

$$\kappa_{\perp} = +(q_0^2 - q_{\parallel}^2)^{1/2} \quad \text{for } q_{\parallel} \leq q_0, \quad (4.37)$$

$$\kappa_{\perp} = +i(q_{\parallel}^2 - q_0^2)^{1/2} \quad \text{for } q_{\parallel} > q_0. \quad (4.38)$$

In terms of $\kappa_{\perp}$, (4.36) can be written in the form

$$g(Z; q_{\parallel}, \omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} \frac{e^{iq_{\perp}Z} dq_{\perp}}{(q_{\perp} - \kappa_{\perp})(q_{\perp} + \kappa_{\perp})}. \quad (4.39)$$

The integral in (4.39) can easily be carried out by contour integration in a complex $q_{\perp}$ -plane when $q_{\parallel} > q_0$. In this case, the two first-order poles are situated on the imaginary axis at $q_{\perp} = \pm i(q_{\parallel}^2 - q_0^2)^{1/2}$. For $Z > 0$, the integration is along a closed contour (semicircle) around the pole located in the upper halfplane at $q_{\perp} = \kappa_{\perp}$. The semicircle has its center at the origo, and its rectilinear part coincides with the real $q_{\perp}$ -axis. In the limit where the radius of the semicircle tends to infinity, the contribution to the integral from the curved part of the contour vanishes, and we are left with the integral along the real $q_{\perp}$ -axis. For $Z < 0$, the contour is a semicircle in the lower halfplane around the pole located at $q_{\perp} = -\kappa_{\perp}$. The residue theorem then gives

$$g(Z; q_{\parallel}, \omega) = \frac{1}{2}(q_{\parallel}^2 - q_0^2)^{-1/2} e^{-(q_{\parallel}^2 - q_0^2)^{1/2}|Z|}, \quad q_{\parallel} > q_0 \quad (4.40)$$

for both $Z > 0$ and $Z < 0$. The Huygens propagator $g(Z; q_{\parallel}, \omega)$ hence decays exponentially (with a decay constant $(q_{\parallel}^2 - q_0^2)^{1/2}$), with the distance from the $Z = 0$ plane. For $q_{\parallel} < q_0$, the two first-order poles ly on the real axis at $q_{\perp} = \pm(q_0^2 - q_{\parallel}^2)^{1/2}$. In this case, the integral is undefined until we specify the contour of integration. The specification is done guided by physical principles. Since one wants to retain only outgoing fields from the source plane $z' = \text{constant}$ (see Sect. 2.3), the closed contour is chosen so that only one of the poles is inside the contour. For $Z > 0$, the contour consists of a semicircle (with infinite radius) in the

upper halfplane, a small almost closed circle (with infinitely small radius) around the pole, located at $\kappa_{\perp}$ and two straight line sections parallel to the real $q_{\perp}$ -axis (an infinitely small distance above). For $Z < 0$, the contour is around the pole at $q_{\perp} = -\kappa_{\perp}$ and closed from below. With the help of the residue theorem one obtains the result

$$g(Z; \mathbf{q}_{\parallel}, \omega) = \frac{i}{2} (q_0^2 - q_{\parallel}^2)^{-1/2} e^{i(q_0^2 - q_{\parallel}^2)^{1/2} |Z|}, \quad q_{\parallel} < q_0 \quad (4.41)$$

valid for both $Z > 0$ and $Z < 0$. The contours used to determine the integral in (4.39) are shown in Figs. 4.1 and 4.2. After multiplication with $\exp(-i\omega t)$, cf. (4.3), it appears that the Huygens propagator in (4.41) relates to outgoing undamped plane waves from the source plane $z' = \text{constant}$. By means of the quantity $\kappa_{\perp}$ ((4.37) or (4.38)), (4.40) and (4.41) can be written as one, viz.,

$$g(Z; \mathbf{q}_{\parallel}, \omega) = \frac{i}{2\kappa_{\perp}} e^{i\kappa_{\perp} |Z|}. \quad (4.42)$$

The expression in (4.42) is our final one for the Huygens propagator in the mixed representation. The angular spectrum representation of the scalar propagator $g(R; \omega)$ thus is

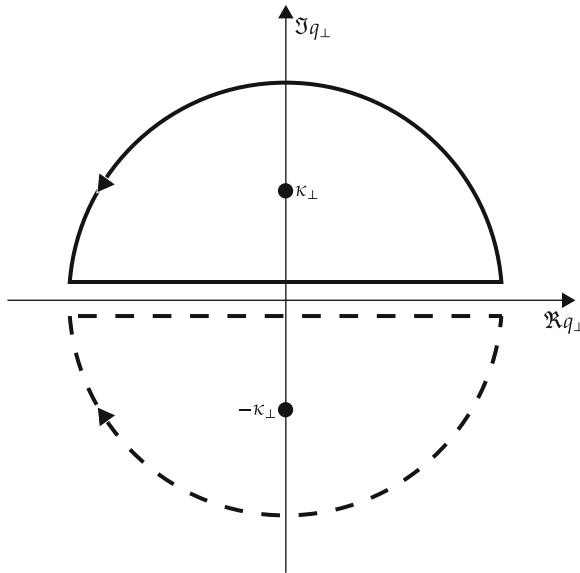


Fig. 4.1 Schematic illustration of the contours which in a complex $q_{\perp}$ -plane are used to determine the scalar propagator in the mixed representation $[g(Z; \mathbf{q}_{\parallel}, \omega)]$ in the case $q_{\parallel} > q_0$. The two first-order poles are located on the imaginary axis at $q_{\perp} = \pm \kappa_{\perp}$, where $\kappa_{\perp} = i(q_{\parallel}^2 - q_0^2)^{1/2}$. The contour in the *upper* halfplane is used for $Z > 0$, and the one in the *lower* halfplane for $Z < 0$

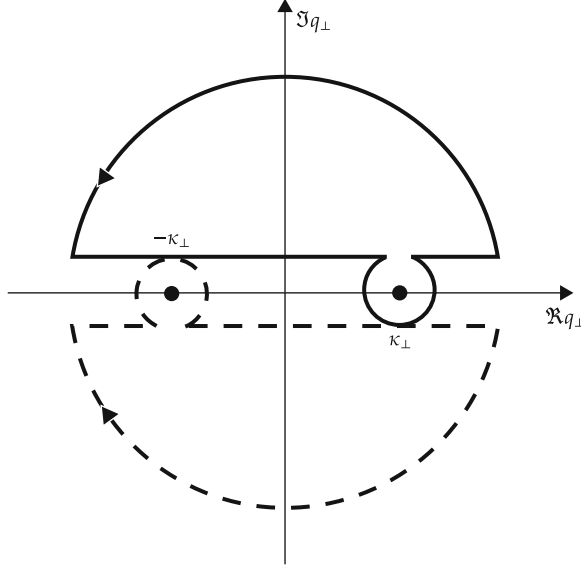


Fig. 4.2 Contours in the complex $q_{\perp}$ -plane used to determine the scalar propagator $g(Z; \mathbf{q}_{\parallel}, \omega)$ when $q_{\parallel} < q_0$. The first-order poles lie on the real axis at $q_{\perp} = \pm \kappa_{\perp}$, where $\kappa_{\perp} = (q_0^2 - q_{\parallel}^2)^{1/2}$. The contour drawn in *full line* is used for $Z > 0$, and the *dashed-line* contour for $Z < 0$

$$g(\mathbf{R}_{\parallel}, Z; \omega) = \frac{i}{8\pi^2} \int_{-\infty}^{\infty} \frac{1}{\kappa_{\perp}} e^{i(\mathbf{q}_{\parallel} \cdot \mathbf{R}_{\parallel} + \kappa_{\perp}|Z|)} d^2 q_{\parallel}, \quad (4.43)$$

where $\mathbf{R}_{\parallel} = X\hat{x} + Y\hat{y}$ with $X = x - x'$ and $Y = y - y'$. The representation in (4.43) is one form of the Weyl representation of a diverging spherical (scalar) wave. The original version of Weyl's representation of $g(\mathbf{R}; \omega)$, obtained in a paper dealing with the propagation of electromagnetic waves over a conducting surface [58], is somewhat more general than the one in (4.43); see Sect. 4.6.

4.3.2 Dyadic Green Function, $G(Z; \mathbf{q}_{\parallel}, \omega)$

In the mixed representation, the integral expression for the Green function for the electric field is given by the dyadic formula

$$\mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} [U - q_0^{-2}(\mathbf{q}_{\parallel} + q_{\perp}\hat{z})(\mathbf{q}_{\parallel} + q_{\perp}\hat{z})] \frac{e^{iq_{\perp}Z} dq_{\perp}}{q_{\perp}^2 + q_{\parallel}^2 - q_0^2}, \quad (4.44)$$

as one realizes by combining (4.20) (with $V(z; \mathbf{q}_{\parallel}, \omega)$ replaced by $\mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega)$), (4.21), and (4.30). The integration in (4.44) can be carried out using contour integration in a similar fashion as was done for the scalar propagator in Sect. 4.3.1 [50],

but with the knowledge of the explicit expression for $g(Z; \mathbf{q}_{\parallel}, \omega)$, it is easier to use the relation

$$\mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega) = \left(U + \frac{1}{q_0^2} \mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \right) g(Z; \mathbf{q}_{\parallel}, \omega), \quad (4.45)$$

with $\mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right)$ given by (4.4). Since

$$\frac{\partial}{\partial z} e^{i\kappa_{\perp}|Z|} = i\kappa_{\perp} e^{i\kappa_{\perp}|Z|} \text{sgn} Z, \quad (4.46)$$

where $\text{sgn} Z = +1$ for $Z > 0$ and $\text{sgn} Z = -1$ for $Z < 0$, one immediately obtains the result

$$\begin{aligned} \mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega) = \frac{i}{2\kappa_{\perp} q_0^2} e^{i\kappa_{\perp}|Z|} \left[q_0^2 \mathbf{U} - \mathbf{q}_{\parallel} \mathbf{q}_{\parallel} - \kappa_{\perp}^2 \hat{\mathbf{z}} \hat{\mathbf{z}} \right. \\ \left. - (\mathbf{q}_{\parallel} \hat{\mathbf{z}} + \hat{\mathbf{z}} \mathbf{q}_{\parallel}) \kappa_{\perp} \text{sgn} Z \right]. \end{aligned} \quad (4.47)$$

If wished, the reader may insert the dyadic expression

$$\mathbf{U} = \hat{\mathbf{q}}_{\parallel} \hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{z}} \times \hat{\mathbf{q}}_{\parallel} \hat{\mathbf{q}}_{\parallel} \times \hat{\mathbf{z}} + \hat{\mathbf{z}} \hat{\mathbf{z}} \quad (4.48)$$

for the unit tensor into (4.47).

4.3.3 Dyadic Green function, $\mathbf{G}_{\text{M}}(Z; \mathbf{q}_{\parallel}, \omega)$

In consequence of (3.31), the dyadic Green function for the magnetic field can be obtained from the formula

$$\mathbf{G}_{\text{M}}(Z; \mathbf{q}_{\parallel}, \omega) = (iq_0)^{-1} \mathbf{U} \times \mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) g(Z; \mathbf{q}_{\parallel}, \omega). \quad (4.49)$$

With $\mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right)$ given by (4.4), and by use of (4.46) one readily gets

$$\mathbf{G}_{\text{M}}(Z; \mathbf{q}_{\parallel}, \omega) = \frac{i}{2\kappa_{\perp} q_0} e^{i\kappa_{\perp}|Z|} \mathbf{U} \times (\mathbf{q}_{\parallel} + \kappa_{\perp} \hat{\mathbf{z}} \text{sgn} Z), \quad (4.50)$$

possible with the expression in (4.48) for $\mathbf{U}$ inserted, and cross products of vectors calculated. In the mixed representation, the Green functions for the electric and magnetic fields are related as follows:

$$\mathbf{G}_M(Z; \mathbf{q}_\parallel, \omega) = (iq_0)^{-1} \mathcal{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_\parallel \right) \times \mathbf{G}(Z; \mathbf{q}_\parallel, \omega), \quad (4.51)$$

cf. (3.28), (4.4), and (4.5).

4.4 Evanescent Electromagnetic Fields

4.4.1 Electromagnetic Fields from a Sheet Source

In the mixed representation, the electric field, $\mathbf{E}(z; \mathbf{q}_\parallel, \omega)$, from a current density distribution, $\mathbf{J}(z; \mathbf{q}_\parallel, \omega)$, is outside the distribution given by

$$\mathbf{E}(z; \mathbf{q}_\parallel, \omega) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}(z - z'; \mathbf{q}_\parallel, \omega) \cdot \mathbf{J}(z'; \mathbf{q}_\parallel, \omega) dz', \quad (4.52)$$

where

$$\mathbf{G}(Z; \mathbf{q}_\parallel, \omega) = \mathbf{\Gamma}(\text{sgn}Z; \mathbf{q}_\parallel, \omega) e^{i\kappa_\perp |Z|} \quad (4.53)$$

with

$$\mathbf{\Gamma}(\text{sgn}Z; \mathbf{q}_\parallel, \omega) = \frac{i}{2q_0^2 \kappa_\perp} [q_0^2 \mathbf{U} - \mathbf{q}_\parallel \mathbf{q}_\parallel - \kappa_\perp^2 \hat{z} \hat{z} - (\mathbf{q}_\parallel \hat{z} + \hat{z} \mathbf{q}_\parallel) \kappa_\perp \text{sgn}Z]; \quad (4.54)$$

see (4.47). Let us now assume that the source current density is nonvanishing only on a plane sheet located at $z' = z_0$. Thus,

$$\mathbf{J}(z'; \mathbf{q}_\parallel, \omega) = \mathbf{J}_0(\mathbf{q}_\parallel, \omega) \delta(z' - z_0), \quad (4.55)$$

and consequently

$$\mathbf{E}(z; \mathbf{q}_\parallel, \omega) = i\mu_0\omega \mathbf{\Gamma}(\text{sgn}(z - z_0); \mathbf{q}_\parallel, \omega) \cdot \mathbf{J}_0(\mathbf{q}_\parallel, \omega) e^{i\kappa_\perp |z - z_0|}. \quad (4.56)$$

Together, (4.37), (4.38), and (4.56) show that the field for a *given* $\mathbf{q}_\parallel$ for which $q_\parallel < q_0$ consists of two spatially nondecaying so-called homogeneous plane waves propagating *away* from the sheet into the two halfspaces $z > z_0$ and $z < z_0$. The real wave vectors of these waves are given by $\mathbf{q}_\parallel + \hat{z}(q_0^2 - q_\parallel^2)^{1/2}$ ($z > z_0$) and $\mathbf{q}_\parallel - \hat{z}(q_0^2 - q_\parallel^2)^{1/2}$ ($z < z_0$). For $q_\parallel > q_0$, the field consists of two so-called inhomogeneous plane waves. The two waves have the same (and real) wave vectors parallel to the sheet plane, namely $\mathbf{q}_\parallel$, but decay exponentially along the z -axis *away* from the sheet with the same decay constant $(q_\parallel^2 - q_0^2)^{1/2}$. These inhomogeneous waves, with the complex wave vector $\mathbf{q}_\parallel + i(q_\parallel^2 - q_0^2)^{1/2} \hat{z}$ ($z > z_0$) and $\mathbf{q}_\parallel - i(q_\parallel^2 - q_0^2)^{1/2} \hat{z}$ ($z < z_0$) often are called evanescent waves. The word *evanescent* originates in the Latin word *evanesco* which has the meanings *fades away* or *loses power*.

(or *taste*, or *interest*). Despite the translation $\text{evanesco} \Leftrightarrow \text{loses interest}$, evanescent waves are of great importance in near-field electrodynamics!

From the integral relation

$$\mathbf{B}(z; \mathbf{q}_{\parallel}, \omega) = \frac{i\mu_0\omega}{c_0} \int_{-\infty}^{\infty} \mathbf{G}_M(z - z'; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}(z'; \mathbf{q}_{\parallel}, \omega) dz', \quad (4.57)$$

where, for field points in vacuum (see (4.50))

$$\mathbf{G}_M(Z; \mathbf{q}_{\parallel}, \omega) = \mathbf{\Gamma}_M(\text{sgn}Z; \mathbf{q}_{\parallel}, \omega) e^{i\kappa_{\perp}|Z|} \quad (4.58)$$

with

$$\mathbf{\Gamma}_M(\text{sgn}Z; \mathbf{q}_{\parallel}, \omega) = \frac{i}{2q_0\kappa_{\perp}} \mathbf{U} \times (\mathbf{q}_{\parallel} + \hat{\mathbf{z}}\kappa_{\perp}\text{sgn}Z), \quad (4.59)$$

one obtains the expression

$$\mathbf{B}(z; \mathbf{q}_{\parallel}, \omega) = \frac{i\mu_0\omega}{c_0} \mathbf{\Gamma}_M(\text{sgn}(z - z_0); \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}_0(\mathbf{q}_{\parallel}, \omega) e^{i\kappa_{\perp}|z - z_0|} \quad (4.60)$$

for the magnetic field from the source current density given in (4.55). The discussion of the homogeneous and inhomogeneous plane waves for the $\mathbf{B}$ -field parallels the one for the $\mathbf{E}$ -field, of course.

4.4.2 Transfer Matrices

The formula in (4.56) allows one to relate the electric field in one plane $z = z_1$ to the electric field in another plane $z = z_2$ without pre-knowledge of the sheet current density amplitude, $\mathbf{J}_0(\mathbf{q}_{\parallel}, \omega)$. This is not surprising since we deal with fields in vacuum. We do need to know, however, the location of the sheet, i.e., the z_0 -coordinate, if the two planes $z = z_1$ and $z = z_2$ are located on opposite sides of the sheet. Elementary calculations lead to the result

$$\mathbf{E}(z_2; \mathbf{q}_{\parallel}, \omega) = \mathbf{T}(z_0, z_1, z_2; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{E}(z_1; \mathbf{q}_{\parallel}, \omega), \quad (4.61)$$

where the so-called transfer matrix, $\mathbf{T}(z_0, z_1, z_2; \mathbf{q}_{\parallel}, \omega)$, is given by

$$\mathbf{T}(z_0, z_1, z_2; \mathbf{q}_{\parallel}, \omega) = \begin{cases} e^{i\kappa_{\perp}(z_2 - z_1)} \mathbf{U}, & z_1, z_2 > z_0 \\ e^{i\kappa_{\perp}(z_1 - z_2)} \mathbf{U}, & z_1, z_2 < z_0 \\ e^{i\kappa_{\perp}(z_1 + z_2 - 2z_0)} \mathbf{\Gamma}(+1; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{\Gamma}^{-1}(-1; \mathbf{q}_{\parallel}, \omega), & z_1 < z_0, z_2 > z_0 \\ e^{i\kappa_{\perp}(2z_0 - z_1 - z_2)} \mathbf{\Gamma}(-1; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{\Gamma}^{-1}(+1; \mathbf{q}_{\parallel}, \omega), & z_1 > z_0, z_2 < z_0. \end{cases} \quad (4.62)$$

The transfer matrix is a useful concept for many applications in near-field optics, e.g., for near-field tomography [163]. For a general introduction to diffraction tomography see [43].

4.4.3 Mixed Current Density of a Moving Point Charge

In our discussion of the angular spectrum representation, we have so far not made any specification of the current density in the mixed representation. Let us now assume that the current density is that of a single point-particle. Generalization to an arbitrary number of point-particles is straightforward. Using the notation of (2.33), the current density of the particle is given by

$$\mathbf{J}(\mathbf{r}; \omega) = Q \int_{-\infty}^{\infty} \mathbf{v}_Q(t) \delta(\mathbf{r} - \mathbf{r}_Q(t)) e^{i\omega t} dt \quad (4.63)$$

in the spectral representation, cf. (3.56). Since

$$\delta(\mathbf{r} - \mathbf{r}_Q(t)) = \delta(\mathbf{r} - \mathbf{r}_Q^{\parallel}(t)) \delta(z - z_Q(t)), \quad (4.64)$$

where $\mathbf{r}_Q^{\parallel}(t) = x_Q(t)\hat{\mathbf{x}} + y_Q(t)\hat{\mathbf{y}}$ is the component at time $t = t$ of the particle position vector perpendicular to the z -axis, the particle current density is given by

$$\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) = Q \int_{-\infty}^{\infty} \mathbf{v}_Q(t) \delta(\mathbf{r}_{\parallel} - \mathbf{r}_Q^{\parallel}(t)) \delta(z - z_Q(t)) e^{i(\omega t - \mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel})} d^2 r_{\parallel} dt \quad (4.65)$$

in the mixed representation. The presence of $\delta(\mathbf{r}_{\parallel} - \mathbf{r}_Q^{\parallel}(t))$ immediately allows one to carry out the two spatial integrations. Thus,

$$\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) = Q \int_{-\infty}^{\infty} \mathbf{v}_Q(t) \delta(z - z_Q(t)) e^{i(\omega t - \mathbf{q}_{\parallel} \cdot \mathbf{r}_Q^{\parallel}(t))} dt. \quad (4.66)$$

If the particle trajectory does not cross the *arbitrarily* chosen z -plane, $\delta(z - z_Q(t)) = 0$ for all t , and the mixed current density will therefore vanish in such planes, of course. If the particle crosses the given z -plane say i times, the times of crossing, t_i , will be given implicitly by the equation

$$z = z_Q(t_i). \quad (4.67)$$

With a knowledge of these times the integration in (4.66) can be carried out with the help of (2.36) generalized to the case where $f(t')$ has i zero points. Hence,

$$\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) = Q \sum_i \frac{\mathbf{v}_Q(t_i)}{|v_{Q,z}(t_i)|} e^{i(\omega t_i - \mathbf{q}_{\parallel} \cdot \mathbf{r}_Q^{\parallel}(t_i))}, \quad (4.68)$$

where $v_{Q,z}(t_i)$ is the z -component of the particle velocity at $t = t_i$. In the mixed representation, the electric and magnetic fields of the moving point particle are obtained by combining (4.67) (for $z = z'$) and (4.68) with (4.52) and (4.57), respectively. The integration over z' is replaced by a sum of integrations over t_i -intervals in which $z' = z_Q(t_i)$ is a monotonically increasing or decreasing function of t_i . In each t_i -interval one has $dz' = v_{Q,z}(t_i)dt_i$, and thus $dz'/|v_{Q,z}(t_i)| = \pm dt_i$.

If the particle motion is confined to a plane $z = z_0$, i.e., $z_Q(t) = z_0$ and $v_Q(t) = v_Q^\parallel(t) = d\mathbf{r}_Q^\parallel(t)/dt$, the current density in (4.66) is reduced to

$$\mathbf{J}(z; \mathbf{q}_\parallel, \omega) = Q \int_{-\infty}^{\infty} v_Q^\parallel(t) e^{i(\omega t - \mathbf{q}_\parallel \cdot \mathbf{r}_Q^\parallel(t))} dt \delta(z - z_0). \quad (4.69)$$

The expression in (4.69) has the form given in (4.55) *provided* the z -component of $\mathbf{J}_0(\mathbf{q}_\parallel, \omega)$ vanishes. *Approximately* one can allow $\mathbf{J}_0(\mathbf{q}_\parallel, \omega)$ to have a nonvanishing z -component in cases where the particle motion is confined to the vicinity of plane $z = z_0$. In these cases $\delta(z - z_Q(t))$ may be replaced by its lowest order Taylor series term $\delta(z - z_0)$.

4.4.4 Cycle-Averaged Field Momentum Density

In this subsection, we shall investigate the field momentum density distribution outside a current sheet. It will be assumed that the sheet carries a monochromatic plane-wave current density, and only cycle-averaged quantities are calculated.

If one first replaces the integration variable ω by Ω in the Fourier integral in (3.3), and then inserts for the Fourier amplitude the monochromatic ansatz

$$\mathbf{V}(\mathbf{r}; \omega) = \pi [V_\omega(\mathbf{r})\delta(\omega - \Omega) + V_\omega^*(\mathbf{r})\delta(\omega + \Omega)], \quad (4.70)$$

one obtains the following form for the monochromatic real vector field:

$$\mathbf{V}(\mathbf{r}, t) = \frac{1}{2} (V_\omega(\mathbf{r}) e^{-i\omega t} + V_\omega^*(\mathbf{r}) e^{i\omega t}). \quad (4.71)$$

By writing the electric, $\mathbf{E}(\mathbf{r}, t)$, and magnetic, $\mathbf{B}(\mathbf{r}, t)$ fields in the form given in (4.71), it is easy to show that the cycle-averaged ($\langle \dots \rangle$) field momentum density is given by

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\epsilon_0}{4} (\mathbf{E}_\omega(\mathbf{r}) \times \mathbf{B}_\omega^*(\mathbf{r}) + \text{c.c.}), \quad (4.72)$$

where c.c. means the complex conjugate of the first term in the parenthesis. By replacing the vectorial integration variable $\mathbf{q}_\parallel$ by $\mathbf{Q}_\parallel$ in (4.2), and inserting afterwards the single plane-wave ansatz

$$V_\omega(z; \mathbf{Q}_\parallel) = (2\pi)^2 V_{\omega, \mathbf{q}_\parallel}(z) \delta(\mathbf{q}_\parallel - \mathbf{Q}_\parallel), \quad (4.73)$$

one gets

$$V_{\omega}(\mathbf{r}) = V_{\omega, \mathbf{q}_{\parallel}}(z) e^{i \mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel}}. \quad (4.74)$$

By using such a form for $E_{\omega}(\mathbf{r})$ and $B_{\omega}(\mathbf{r})$, (4.72) is reduced to

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\epsilon_0}{4} \left(E_{\omega, \mathbf{q}_{\parallel}}(z) \times B_{\omega, \mathbf{q}_{\parallel}}^*(z) + \text{c.c.} \right). \quad (4.75)$$

For a sheet, located at $z = z_0$, the monochromatic plane-wave current density is written in the form

$$\mathbf{J}(\mathbf{r}, t) = \delta(z - z_0) \frac{1}{2} \left[\mathbf{J}_{\omega, \mathbf{q}_{\parallel}}^0 e^{i(\mathbf{q}_{\parallel} \cdot \mathbf{r}_{\parallel} - \omega t)} + \text{c.c.} \right]. \quad (4.76)$$

The electric, $E_{\omega, \mathbf{q}_{\parallel}}(z)$, and magnetic, $B_{\omega, \mathbf{q}_{\parallel}}(z)$, fields in turn are related to $\mathbf{J}_{\omega, \mathbf{q}_{\parallel}}$ as follows, cf. (4.52) and (4.57):

$$E_{\omega, \mathbf{q}_{\parallel}}(z) = i \mu_0 \omega \mathbf{G}(z - z_0; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}_{\omega, \mathbf{q}_{\parallel}}^0, \quad (4.77)$$

$$B_{\omega, \mathbf{q}_{\parallel}}(z) = i \mu_0 \omega c_0^{-1} \mathbf{G}_M(z - z_0; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}_{\omega, \mathbf{q}_{\parallel}}^0. \quad (4.78)$$

Since the tensor $\mathbf{G}(z - z_0; \mathbf{q}_{\parallel}, \omega)$ is symmetric, a combination of (4.75), (4.77) and (4.78) gives a cycle-averaged field momentum density

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\mu_0 \omega^2}{4c_0^3} (\mathbf{J}_0 \cdot \mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega) \times \mathbf{G}_M^*(Z; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}_0^* + \text{c.c.}), \quad (4.79)$$

with the abbreviations $Z = z - z_0$, and $\mathbf{J}_0 = \mathbf{J}_{\omega, \mathbf{q}_{\parallel}}^0$. Using the explicit expressions for the Green functions in the mixed representation ((4.47) and (4.50)) it is a straightforward but tedious matter to calculate $\langle \mathbf{g}(\mathbf{r}, t) \rangle$ as a function of ω , $\mathbf{q}_{\parallel}$, $\mathbf{J}_0$, and $z - z_0$.

Below, I cite and discuss the results for three special cases, namely those where the current density amplitude is (1) parallel to the $\hat{\mathbf{q}}_{\parallel}$ -direction, $\mathbf{J}_0 = A \hat{\mathbf{q}}_{\parallel}$, (2) perpendicular to the $\hat{\mathbf{q}}_{\parallel}$ - $\hat{\mathbf{z}}$ -plane, $\mathbf{J}_0 = B \hat{\mathbf{q}}_{\parallel}^t$, where $\hat{\mathbf{q}}_{\parallel}^t = \hat{\mathbf{z}} \times \hat{\mathbf{q}}_{\parallel}$, and (3) parallel to the $\hat{\mathbf{z}}$ -direction, $\mathbf{J}_0 = C \hat{\mathbf{z}}$. The length of the calculations are a bit reduced if one at the beginning introduces the dyadic form

$$\mathbf{U} = \hat{\mathbf{q}}_{\parallel} \hat{\mathbf{q}}_{\parallel} + \hat{\mathbf{q}}_{\parallel}^t \hat{\mathbf{q}}_{\parallel}^t + \hat{\mathbf{z}} \hat{\mathbf{z}} \quad (4.80)$$

of the unit tensor in the expressions for the Green functions for the electric and magnetic fields. The final result are as follows:

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\mu_0 \omega |A|^2}{16c_0^2} e^{i(\kappa_{\perp} - \kappa_{\perp}^*)|Z|} [2q_{\parallel} \hat{\mathbf{q}}_{\parallel} + \hat{\mathbf{z}}(\kappa_{\perp} + \kappa_{\perp}^*) \text{sgn} Z] \quad (4.81)$$

for $\mathbf{J}_0 = A\hat{\mathbf{q}}_{\parallel}$,

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\mu_0 \omega^3 |B|^2}{16c_0^4 |\kappa_{\perp}|^2} e^{i(\kappa_{\perp} - \kappa_{\perp}^*)|Z|} [2q_{\parallel} \hat{\mathbf{q}}_{\parallel} + \hat{\mathbf{z}}(\kappa_{\perp} + \kappa_{\perp}^*) \text{sgn} Z] \quad (4.82)$$

for $\mathbf{J}_0 = B\hat{\mathbf{q}}_{\parallel}^t = B\hat{\mathbf{z}} \times \hat{\mathbf{q}}_{\parallel}$, and

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle = \frac{\mu_0 \omega q_{\parallel}^2 |C|^2}{16c_0^2 |\kappa_{\perp}|^2} e^{i(\kappa_{\perp} - \kappa_{\perp}^*)|Z|} [2q_{\parallel} \hat{\mathbf{q}}_{\parallel} + \hat{\mathbf{z}}(\kappa_{\perp} + \kappa_{\perp}^*) \text{sgn} Z] \quad (4.83)$$

for $\mathbf{J}_0 = C\hat{\mathbf{z}}$. One notices that the directions of the cycle-averaged momenta, as well as the dependences of these as a function of the distance from the sheet, are the same in the three cases. If the two plane waves are homogeneous the cycle-averaged momentum distribution must be independent of the distance $|Z|$ from the sheet. This indeed follows from (4.81)–(4.83) since $\kappa_{\perp}$ is real for a homogeneous wave; see (4.37). For the homogeneous waves, the directions of $\langle \mathbf{g}(\mathbf{r}, t) \rangle$ in the two halfplanes are given by the unit vectors $(\hat{\mathbf{q}}_{\parallel} + \hat{\mathbf{z}}\kappa_{\perp} \text{sgn} Z)/(1 + \kappa_{\perp}^2)^{1/2}$, not unexpectedly. If $q_{\parallel} = 0$, the current density will be the same everywhere in the sheet at a given time, and if furthermore the current density points in a direction normal to the sheet plane ($\mathbf{J}_0 = C\hat{\mathbf{z}}$), $\langle \mathbf{g}(\mathbf{r}, t) \rangle$ must vanish. That this is indeed the case appears from (4.83) setting $q_{\parallel} = 0$. For $q_{\parallel} = 0$, $\langle \mathbf{g}(\mathbf{r}, t) \rangle$ must for symmetry reasons also be the same for the cases $\mathbf{J}_0 = A\hat{\mathbf{q}}_{\parallel}$ and $\mathbf{J}_0 = B\hat{\mathbf{q}}_{\parallel}^t$ when $A = B$. This result follows readily by a comparison of (4.81) and (4.82), since $|\kappa_{\perp}| = q_0 = \omega/c_0$ for $q_{\parallel} = 0$. The cycle-averaged Poynting vector, $\langle \mathbf{S}(\mathbf{r}, t) \rangle$, is readily obtained for the three cases, remembering that $\langle \mathbf{S}(\mathbf{r}, t) \rangle = c_0^2 \langle \mathbf{g}(\mathbf{r}, t) \rangle$; see (2.120).

For the evanescent waves fulfilling $q_{\parallel} > q_0$, and thus $\kappa_{\perp} = i(q_{\parallel}^2 - q_0^2)^{1/2}$ (4.38) one has $\kappa_{\perp} + \kappa_{\perp}^* = 0$. This implies that the time-averaged field momentum is parallel to the sheet plane, and in the direction given by $\hat{\mathbf{q}}_{\parallel}$, in all three cases. It can be shown from (4.79) that this well known result holds in general, i.e., independent of $\mathbf{J}_0$. Although there is no cycle-averaged momentum (and hence energy flow) component in the direction perpendicular to the sheet-plane, there still is a nonvanishing cycle-averaged field energy density outside the sheet. This is easy to prove starting from (2.113), and remembering that $\kappa_{\perp} = i(q_{\parallel}^2 - q_0^2)^{1/2}$. It turns out that $\langle W(\mathbf{r}, t) \rangle$ decays exponentially with the distance from the sheet, i.e., $\langle W(\mathbf{r}, t) \rangle \sim \exp[-2(q_{\parallel}^2 - q_0^2)^{1/2}|Z|]$. The cycle-averaged momentum also exhibits this $|Z|$ -dependence for the evanescent waves, an expected result because $\langle W \rangle = c_0^{-1} |\langle \mathbf{S} \rangle| = c_0 |\langle \mathbf{g} \rangle|$. In the three special cases in (4.81)–(4.83) the cycle-averaged momenta for evanescent (Evan) fields, $\kappa_{\perp} - \kappa_{\perp}^* = 2i(q_{\parallel}^2 - q_0^2)^{1/2}$, are given by

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle_{\text{Evan}} = \frac{\mu_0 \omega q_{\parallel} |A|^2}{8c_0^2} \hat{\mathbf{q}}_{\parallel} e^{-2(q_{\parallel}^2 - q_0^2)^{1/2} |Z|}, \quad (4.84)$$

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle_{\text{Evan}} = \frac{\mu_0 \omega^3 q_{\parallel} |B|^2}{8c_0^4 (q_{\parallel}^2 - q_0^2)} \hat{\mathbf{q}}_{\parallel} e^{-2(q_{\parallel}^2 - q_0^2)^{1/2} |Z|}, \quad (4.85)$$

$$\langle \mathbf{g}(\mathbf{r}, t) \rangle_{\text{Evan}} = \frac{\mu_0 \omega q_{\parallel}^3 |C|^2}{8c_0^2 (q_{\parallel}^2 - q_0^2)} \hat{\mathbf{q}}_{\parallel} e^{-2(q_{\parallel}^2 - q_0^2)^{1/2} |Z|}, \quad (4.86)$$

remembering that $q_{\parallel} > q_0$.

4.5 Nonretarded ($c_0 \rightarrow \infty$) Electrodynamics in Vacuum

It is often possible to treat the electrodynamic interaction between charged particles in close contact as nonretarded. In the nonretarded limit, the fundamental set of electrodynamic equations take a particularly simple form, and a neglect of the finite propagation speed of light can often be justified in near-field electrodynamics. In the present section, we shall briefly study the nonretarded electromagnetic fields as they appear in the mixed representation, and thereafter the field equations they obey in vacuum. The Green function formalism is a good starting point for the analysis because the dyadic Green functions for the electric and magnetic field asymptotically, i.e., for $c_0 \rightarrow \infty$, relate directly to the nonretarded fields.

If formally one lets $c_0 \rightarrow \infty$, the Green function for the electric field (4.47) is reduced to the form

$$\begin{aligned} \mathbf{G}(Z; \mathbf{q}_{\parallel}, \omega | c_0 \rightarrow \infty) &\equiv \mathbf{G}^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) \\ &= \frac{q_{\parallel}}{2q_0^2} e^{-q_{\parallel} |Z|} [\hat{\mathbf{z}}\hat{\mathbf{z}} - \hat{\mathbf{q}}_{\parallel}\hat{\mathbf{q}}_{\parallel} - i(\hat{\mathbf{q}}_{\parallel}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{q}}_{\parallel}) \text{sgn} Z], \end{aligned} \quad (4.87)$$

since $\kappa_{\perp} \rightarrow i q_{\parallel}$ for $c_0 \rightarrow \infty$; see (4.38). In view of the subsequent calculations it is useful to write (4.87) in the alternative dyadic form

$$\mathbf{G}^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) = \frac{q_{\parallel}}{2q_0^2} e^{-q_{\parallel} |Z|} (i\hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{z}} \text{sgn} Z)(i\hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{z}} \text{sgn} Z). \quad (4.88)$$

For $c_0 \rightarrow \infty$, the Green function for the magnetic field (4.50) becomes

$$\begin{aligned} \mathbf{G}_M(Z; \mathbf{q}_{\parallel}, \omega | c_0 \rightarrow \infty) &\equiv \mathbf{G}_M^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) \\ &= \frac{1}{2i q_0} e^{-q_{\parallel} |Z|} \mathbf{U} \times (i\hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{z}} \text{sgn} Z). \end{aligned} \quad (4.89)$$

The Green functions $\mathbf{G}^{\infty}$ and $\mathbf{G}_M^{\infty}$ thus decrease exponentially with a decay constant $q_{\parallel}$ as a function of $|Z|$. It appears from (4.4) and (4.46) that the vectorial

operator $\mathbf{O}$ can be replaced by

$$\mathbf{O}\left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} | c_0 \rightarrow \infty\right) \equiv \mathbf{O}^{\infty}(Z; \mathbf{q}_{\parallel}) = q_{\parallel}(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z) \quad (4.90)$$

when it operates on the Green functions $\mathbf{G}^{\infty}$ and $\mathbf{G}_M^{\infty}$. From (4.88) and (4.90) it now follows that both the scalar and vector product of $\mathbf{O}^{\infty}$ and $\mathbf{G}^{\infty}$ vanish, i.e.,

$$\mathbf{O}^{\infty}(Z; \mathbf{q}_{\parallel}) \cdot \mathbf{G}^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) = \mathbf{O}, \quad (4.91)$$

$$\mathbf{O}^{\infty}(Z; \mathbf{q}_{\parallel}) \times \mathbf{G}^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) = \mathbf{O}. \quad (4.92)$$

To obtain the scalar and vector products of the operator $\mathbf{O}^{\infty}$ with the asymptotic Green function for the magnetic field (4.89), one first make use of (4.80) to rewrite the product $\mathbf{U} \times (i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z)$. Hence,

$$\begin{aligned} \mathbf{U} \times (i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z) &= (i\hat{z} + \hat{\mathbf{q}}_{\parallel} \text{sgn}Z)\hat{\mathbf{q}}_{\parallel}^t - \hat{\mathbf{q}}_{\parallel}^t(i\hat{z} + \hat{\mathbf{q}}_{\parallel} \text{sgn}Z) \\ &= -i \text{sgn} Z [(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z)\hat{\mathbf{q}}_{\parallel}^t - \hat{\mathbf{q}}_{\parallel}^t(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z)]. \end{aligned} \quad (4.93)$$

The scalar product of $\mathbf{O}^{\infty}$ with $\mathbf{G}_M^{\infty}$ now is readily obtained by combining (4.89), (4.90), and (4.93). Thus, one gets

$$\mathbf{O}^{\infty}(Z; \mathbf{q}_{\parallel}) \cdot \mathbf{G}_M^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) = \mathbf{O}. \quad (4.94)$$

Since

$$\mathbf{O}^{\infty} \times \hat{\mathbf{q}}_{\parallel}^t = -iq_{\parallel} \text{sgn}Z(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z) \quad (4.95)$$

one obtains

$$\mathbf{O}^{\infty} \times \mathbf{U} \times (i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z) = q_{\parallel}(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z)(i\hat{\mathbf{q}}_{\parallel} - \hat{z}\text{sgn}Z), \quad (4.96)$$

and finally from (4.88), (4.89), and (4.96)

$$\mathbf{O}^{\infty}(Z; \mathbf{q}_{\parallel}) \times \mathbf{G}_M^{\infty}(Z; \mathbf{q}_{\parallel}, \omega) = -iq_0 \mathbf{G}^{\infty}(Z; \mathbf{q}_{\parallel}, \omega). \quad (4.97)$$

On the basis of the integral relations in (4.52) and (4.57), and the scalar and vector products in (4.91), (4.92), (4.94), and (4.97), one may show that the electric and magnetic fields in the mixed representation in the nonretarded limit, viz.,

$$\mathbf{E}(z; \mathbf{q}_{\parallel}, \omega | c_0 \rightarrow \infty) \equiv \mathbf{E}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}^{\infty}(z - z'; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}(z'; \mathbf{q}_{\parallel}, \omega) dz', \quad (4.98)$$

$$\mathbf{B}(z; \mathbf{q}_{\parallel}, \omega | c_0 \rightarrow \infty) \equiv \mathbf{B}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = \frac{i\mu_0\omega}{c_0} \int_{-\infty}^{\infty} \mathbf{G}_M^{\infty}(z - z'; \mathbf{q}_{\parallel}, \omega) \cdot \mathbf{J}(z'; \mathbf{q}_{\parallel}, \omega) dz', \quad (4.99)$$

satisfy the following set of dynamical equations *in vacuum*:

$$\mathbf{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \times \mathbf{E}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = \mathbf{0}, \quad (4.100)$$

$$\mathbf{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \cdot \mathbf{E}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = 0, \quad (4.101)$$

$$\mathbf{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \times \mathbf{B}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = -\frac{i\omega}{c_0^2} \mathbf{E}^{\infty}(z; \mathbf{q}_{\parallel}, \omega), \quad (4.102)$$

$$\mathbf{O} \left(\frac{\partial}{\partial z}; \mathbf{q}_{\parallel} \right) \cdot \mathbf{B}^{\infty}(z; \mathbf{q}_{\parallel}, \omega) = 0. \quad (4.103)$$

If one compares (4.100)–(4.103) to the vacuum form of the general Maxwell–Lorentz equations ((4.6)–(4.9) with $\rho = 0$ and $\mathbf{J} = \mathbf{0}$) it appears that the two sets are form-identical provided the term $i\omega \mathbf{B}(z; \mathbf{q}, \omega)$ in (4.6) is neglected. We can elaborate on this point by transforming (4.100)–(4.103) back to the space–frequency domain. By remembering the prescription in (4.5) one obtain immediately

$$\nabla \times \mathbf{E}^{\infty}(\mathbf{r}; \omega) = \mathbf{0}, \quad (4.104)$$

$$\nabla \cdot \mathbf{E}^{\infty}(\mathbf{r}; \omega) = 0, \quad (4.105)$$

$$\nabla \times \mathbf{B}^{\infty}(\mathbf{r}; \omega) = -\frac{i\omega}{c_0^2} \mathbf{E}^{\infty}(\mathbf{r}; \omega), \quad (4.106)$$

$$\nabla \cdot \mathbf{B}^{\infty}(\mathbf{r}; \omega) = 0. \quad (4.107)$$

The nonretarded electric field hence is both divergence-free and rotational-free in vacuum, and we shall realize later on that this field varies as R^{-3} with the source-observation distance R . The nonretarded magnetic field varies as R^{-2} , and since $\nabla \times \mathbf{E}^{\infty}$ varies as R^{-4} it is correct to neglect the right side of (3.5) in the nonretarded limit, cf. (4.104). In (3.7) both $\nabla \times \mathbf{B}$ and $i\omega c_0^{-2} \mathbf{E}$ vary as R^{-3} in the limit $c_0 \rightarrow \infty$, and both terms must therefore be kept in the nonretarded limit; cf. (4.106).

4.6 Weyl Representation of the Green Functions

4.6.1 Integrals Over Propagating and Evanescent Waves

In the Weyl expansion of the scalar propagator (4.43) enters an integral over the entire $\mathbf{q}_{\parallel}$ -plane. This double integration is now described in polar coordinates $(\alpha, q_{\parallel}) : q_{\parallel,x} = q_{\parallel} \cos \alpha, q_{\parallel,y} = q_{\parallel} \sin \alpha$. Letting the $q_{\parallel,x}$ -axis coincide with the $\hat{\mathbf{R}}_{\parallel}$ -direction one obtains

$$g(R_{\parallel}, Z; \omega) = \frac{i}{8\pi^2} \int_0^{\infty} \int_0^{2\pi} \frac{1}{\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} e^{iq_{\parallel}R_{\parallel} \cos \alpha} q_{\parallel} d\alpha dq_{\parallel}. \quad (4.108)$$

The integral representation of the Bessel function of the first kind and n th order (n is a natural number), viz.,

$$J_n(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ni\theta + iz \sin \theta} d\theta \quad (4.109)$$

shows that the angular integral in (4.108) can be expressed in terms of

$$J_0(z) = \frac{1}{2\pi} \int_0^{2\pi} e^{iz \cos \alpha} d\alpha. \quad (4.110)$$

Thus,

$$g(R_{\parallel}, Z; \omega) = \frac{i}{4\pi} \int_0^{\infty} \frac{q_{\parallel}}{\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} J_0(q_{\parallel} R_{\parallel}) dq_{\parallel}. \quad (4.111)$$

Now, the Huygens propagator can readily be written as a sum of two integrals, i.e.,

$$\begin{aligned} g(R_{\parallel}, Z; \omega) &= \frac{i}{4\pi} \int_0^{q_0} \frac{q_{\parallel}}{(q_0^2 - q_{\parallel}^2)^{1/2}} e^{i(q_0^2 - q_{\parallel}^2)^{1/2}|Z|} J_0(q_{\parallel} R_{\parallel}) dq_{\parallel} \\ &+ \frac{1}{4\pi} \int_{q_0}^{\infty} \frac{q_{\parallel}}{(q_{\parallel}^2 - q_0^2)^{1/2}} e^{-i(q_{\parallel}^2 - q_0^2)^{1/2}|Z|} J_0(q_{\parallel} R_{\parallel}) dq_{\parallel}, \end{aligned} \quad (4.112)$$

where the first represents the contribution from all propagating modes, and the second the contribution from the evanescent modes.

To obtain in the Weyl representation of the dyadic Green function for the magnetic field the integral contributions from the entire spectra of propagating and evanescent modes we write the Cartesian components of the tensor

$$\mathbf{U} \times (\mathbf{q}_{\parallel} + \kappa_{\perp} \hat{\mathbf{z}} \text{sgn} Z) = (\hat{\mathbf{z}} \hat{\mathbf{q}}_{\parallel}^t - \hat{\mathbf{q}}_{\parallel}^t \hat{\mathbf{z}}) q_{\parallel} + (\hat{\mathbf{q}}_{\parallel}^t \hat{\mathbf{q}}_{\parallel} - \hat{\mathbf{q}}_{\parallel} \hat{\mathbf{q}}_{\parallel}^t) \kappa_{\perp} \text{sgn} Z \quad (4.113)$$

in polar coordinates. With $\hat{\mathbf{q}}_{\parallel} = \hat{\mathbf{x}} \cos \alpha + \hat{\mathbf{y}} \sin \alpha$, and thus $\hat{\mathbf{q}}_{\parallel}^t = -\hat{\mathbf{x}} \sin \alpha + \hat{\mathbf{y}} \cos \alpha$, one obtains after some elementary algebraic calculations

$$\mathbf{U} \times (\mathbf{q}_{\parallel} + \kappa_{\perp} \hat{\mathbf{z}} \text{sgn} Z) = \begin{pmatrix} 0 & -\kappa_{\perp} \text{sgn} Z & q_{\parallel} \sin \alpha \\ \kappa_{\perp} \text{sgn} Z & 0 & -q_{\parallel} \cos \alpha \\ -q_{\parallel} \sin \alpha & q_{\parallel} \cos \alpha & 0 \end{pmatrix}. \quad (4.114)$$

With $\mathbf{G}_M(Z; \mathbf{q}_{\parallel}, \omega)$ given by (4.50), the Weyl expansion of the Green function for the magnetic field thus takes the form (for $Z \neq 0$)

$$\mathbf{G}_M(R_{\parallel}, Z; \omega) = \frac{i}{8\pi^2 q_0} \int_0^\infty \int_0^{2\pi} \frac{q_{\parallel}}{\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} e^{iq_{\parallel}R_{\parallel}\cos\alpha} \begin{pmatrix} 0 & -\kappa_{\perp}\operatorname{sgn}Z & q_{\parallel}\sin\alpha \\ \kappa_{\perp}\operatorname{sgn}Z & 0 & -q_{\parallel}\cos\alpha \\ -q_{\parallel}\sin\alpha & q_{\parallel}\cos\alpha & 0 \end{pmatrix} d\alpha dq_{\parallel}. \quad (4.115)$$

The angular integrations for the (x, z) and (z, x) components yield zero, and the remaining integrals can be expressed in terms of the Bessel functions $J_0(q_{\parallel}R_{\parallel})$ and

$$J_1(z) = \frac{1}{2\pi i} \int_0^{2\pi} \cos\alpha e^{iz\cos\alpha} d\alpha. \quad (4.116)$$

The integral expression given in (4.116) for $J_1(z)$ follows after some straightforward calculations from the general integral representation in (4.109). Hence, one finally obtains

$$\mathbf{G}_M(R_{\parallel}, Z; \omega) = \frac{i}{4\pi q_0} \int_0^\infty \frac{q_{\parallel}}{\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} \begin{pmatrix} 0 & -\kappa_{\perp}J_0(q_{\parallel}R_{\parallel})\operatorname{sgn}Z & 0 \\ \kappa_{\perp}J_0(q_{\parallel}R_{\parallel})\operatorname{sgn}Z & 0 & -iq_{\parallel}J_1(q_{\parallel}R_{\parallel}) \\ 0 & iq_{\parallel}J_1(q_{\parallel}R_{\parallel}) & 0 \end{pmatrix} dq_{\parallel}. \quad (4.117)$$

The division of the integral in (4.117) into integral contributions from propagating and evanescent modes parallels the division of the Huygens propagator.

To express the dyadic Green function for the electric field as an integral over the magnitude of the two-dimensional wave vector $\mathbf{q}_{\parallel}$ one needs the integral expression for the Bessel function of the first kind and second order. From (4.109) one can establish the integral representation

$$J_2(z) = -\frac{1}{2\pi} \int_0^{2\pi} \cos 2\alpha e^{iz\cos\alpha} d\alpha. \quad (4.118)$$

It is left to the reader to carry out the calculations for $\mathbf{G}(R_{\parallel}, Z; \omega)$. The final result is

$$\mathbf{G}(R_{\parallel}, Z; \omega) = \frac{i}{4\pi q_0^2} \int_0^\infty \frac{q_{\parallel}}{\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} \times \begin{pmatrix} q_0^2 J_0(q_{\parallel}R_{\parallel}) & 0 & -i\kappa_{\perp}q_{\parallel}J_1(q_{\parallel}R_{\parallel})\operatorname{sgn}Z \\ -\frac{q_{\parallel}^2}{2}(J_0(q_{\parallel}R_{\parallel}) - J_2(q_{\parallel}R_{\parallel})) & & \\ 0 & q_0^2 J_0(q_{\parallel}R_{\parallel}) & 0 \\ & -\frac{q_{\parallel}^2}{2}(J_0(q_{\parallel}R_{\parallel}) + J_2(q_{\parallel}R_{\parallel})) & \\ -i\kappa_{\perp}q_{\parallel}J_1(q_{\parallel}R_{\parallel})\operatorname{sgn}Z & 0 & q_{\parallel}^2 J_0(q_{\parallel}R_{\parallel}) \end{pmatrix} dq_{\parallel}. \quad (4.119)$$

A comparison of (4.117) and (4.119) shows that the nonvanishing tensor components of $\mathbf{G}_M$ appear in places where the $\mathbf{G}$ -tensor has zeros. We emphasize again that the Green function tensors are written in a coordinate system where $\hat{\mathbf{R}}_{\parallel} = \hat{\mathbf{x}}$.

4.6.2 Integrals Over Generalized Inhomogeneous Waves

In the previous subsection, the integration over the $\mathbf{q}_{\parallel}$ -plane was described in polar coordinates, and with the help of the Bessel functions $J_0(q_{\parallel}R_{\parallel})$, $J_1(q_{\parallel}R_{\parallel})$, and $J_2(q_{\parallel}R_{\parallel})$ it was possible to express the Weyl representations of the various Green functions as a single integral over the magnitude of $\mathbf{q}_{\parallel}$. By this approach an important freedom is lost, however, as we now shall realize.

It appears from (4.47) and (4.50) that the Weyl representations of the Green functions for the electric and magnetic fields have the generic form

$$V(\mathbf{R}; \omega) = (2\pi)^{-2} \int_{-\infty}^{\infty} \frac{i}{2\kappa_{\perp}} e^{i\kappa_{\perp}|Z|} V_0(\text{sgn}Z; \mathbf{q}_{\parallel}, \omega) e^{i\mathbf{q}_{\parallel} \cdot \mathbf{R}_{\parallel}} d^2q_{\parallel}. \quad (4.120)$$

The Huygens propagator multiplied by the unit tensor also has this form with $V_0 = U$; see (4.43). If one sets

$$q_{\parallel,x} = q_0 p, \quad q_{\parallel,y} = q_0 q, \quad \kappa_{\perp} = q_0 m, \quad (4.121)$$

equation (4.120) becomes

$$V(\mathbf{R}; \omega) = \frac{i q_0}{8\pi^2} \int_{-\infty}^{\infty} \frac{1}{m} V_0(\text{sgn}Z; q_0 \sqrt{p^2 + q^2}, \omega) e^{i q_0 (pX + qY + m|Z|)} dp dq. \quad (4.122)$$

A different set of integration variables (α, β) now is introduced by setting

$$p = \sin \alpha \cos \beta, \quad q = \sin \alpha \sin \beta, \quad m = \cos \alpha. \quad (4.123)$$

This choice satisfies the condition $p^2 + q^2 + m^2 = 1$, a condition which is required by (4.37), (4.38), and (4.121). For homogeneous waves ($p^2 + q^2 \leq 1$) α and β are the spherical polar angles of their directions of propagation, the polar axis being along the positive z -direction. For the homogeneous waves the variable ranges are

$$0 \leq \alpha < \frac{\pi}{2}, \quad 0 \leq \beta < 2\pi. \quad (4.124)$$

For evanescent waves ($p^2 + q^2 > 1$) m is an imaginary number, and the related complex α is given by $i|m| = \cos \alpha$. Setting

$$\alpha = \frac{\pi}{2} + i\alpha' \quad (4.125)$$

one gets $\exp(\alpha') = (|m|^2 + 1)^{1/2} - |m|$, and from this relation it appears that as a function of $|m|$ ($0 < |m| < \infty$) α' is a monotonically decreasing function with range $0 > \alpha > -\infty$. For the evanescent waves the variable ranges therefore are

$$\Re \alpha = \frac{\pi}{2}, \quad -\infty < \Im \alpha < 0, \quad 0 \leq \beta < 2\pi. \quad (4.126)$$

In the complex α -plane the α -contour thus consists of a horizontal segment C_1 along the real axis ($0 \leq \Re \alpha < \frac{\pi}{2}$), a quarter circle (in the lower halfplane) with infinitesimal small radius and centered at $(\frac{\pi}{2}, 0)$, and a vertical segment C_2 stretching from $\alpha = \frac{\pi}{2}$ to $\alpha = \frac{\pi}{2} - i\infty$. The sections C_1 and C_2 are associated with homogeneous and evanescent waves, respectively. A schematic illustration of the α -contour is shown in Fig. 4.3. The area elements $dpdq$ and $d\alpha d\beta$ are connected via

$$dpdq = \left| \frac{\partial(p, q)}{\partial(\alpha, \beta)} \right| d\alpha d\beta, \quad (4.127)$$

where

$$\frac{\partial(p, q)}{\partial(\alpha, \beta)} = \frac{\partial p}{\partial \alpha} \frac{\partial q}{\partial \beta} - \frac{\partial p}{\partial \beta} \frac{\partial q}{\partial \alpha} \quad (4.128)$$

is the functional determinant (Jacobian) of the transformation. It is easy to show that

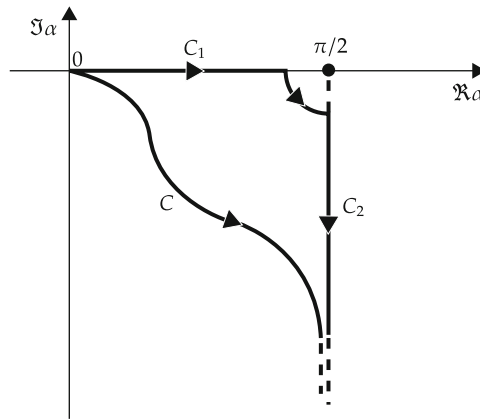


Fig. 4.3 Schematic illustration of contours used in the Weyl polar-angle integral representation of the Green functions for the electric and magnetic fields. As described in the text, the integration variable α is complex, in general. If the integration in the complex α -plane is along the C_1 -quarter circle- C_2 contour a pure division into contributions from homogeneous (propagating) waves and evanescent modes is obtained. The horizontal segment C_1 (along the real axis) is associated with the homogeneous waves, and the vertical section C_2 gives the contribution from the evanescent modes. In the original version of Weyl's representation of a diverging spherical scalar wave a (flexible) contour C is used. With this contour the α -contour integral is over generalized inhomogeneous waves

$$\frac{\partial(p, q)}{\partial(\alpha, \beta)} = m \sin \alpha \quad (4.129)$$

in both the homogeneous and evanescent mode case. In the new variables, the Weyl expansion of $V(\mathbf{R}; \omega)$ in (4.122) is

$$V(\mathbf{R}; \omega) = \frac{iq_0}{8\pi^2} \int_0^{2\pi} \int_{C_1+C_2} V_0(\text{sgn}Z; q_0 \sin \alpha, \omega) \\ \times e^{iq_0(X \sin \alpha \cos \beta + Y \sin \alpha \sin \beta + |Z| \cos \alpha)} \sin \alpha d\alpha d\beta. \quad (4.130)$$

Since the integrand $V_0(\text{sgn}Z; q_0 \sin \alpha, \omega)$ has no poles in the complex α -plane for $\mathbf{G}$, $\mathbf{G}_M$, and $g\mathbf{U}$, one can replace the contour $C_1 + C_2$ by a distorted contour C . The contour C must lie in the domain $0 \leq \Re \alpha < \frac{\pi}{2}$, $\Im \alpha < 0$, but can otherwise be any curve beginning at the origin and approaching asymptotically the point $\frac{\pi}{2} - i\infty$; see Fig. 4.3. Along such a contour C each of the three parameters takes on complex values at every point except at the origin. Thus, with the notation $p = p_R + ip_I$, $q = q_R + iq_I$, and $m = m_R + im_I$, it appears from

$$e^{iq_0(pX+qY+m|Z|)} = e^{iq_0(p_RX+q_RY+m_R|Z|)} e^{-q_0(p_IX+q_1Y+m_I|Z|)} \quad (4.131)$$

that the surfaces of constant amplitude and of constant phase in general are distinct. The various inhomogeneous modes used along the C -curve to obtain $V(\mathbf{R}; \omega)$ thus are generalizations of the evanescent modes studied previously in this chapter.

Chapter 5

Multipole Electrodynamics

5.1 Moment Expansion of Localized Current Density Distribution

In mesoscopic electrodynamics, one is interested in the interaction of electromagnetic fields with particle systems of linear extension much less than the typical wavelength(s) of the field. The prevailing current density distribution in the mesoscopic medium can then with advantage often be approximated by a few of the first terms in a so-called moment expansion. This expansion may be obtained starting from the spatial Fourier integral representation of the current density, i.e.,

$$\mathbf{J}(\mathbf{r}, t) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{J}(\mathbf{q}; t) e^{i\mathbf{q} \cdot \mathbf{r}} d^3q, \quad (5.1)$$

and inserting here a Taylor series expansion,

$$\mathbf{J}(\mathbf{q}; t) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{q} \cdot \nabla_{\mathbf{q}})^n \mathbf{J}(\mathbf{0}; t), \quad (5.2)$$

of the $\mathbf{q}$ -space current density around $\mathbf{q} = \mathbf{0}$. Hence, one obtains

$$\mathbf{J}(\mathbf{r}, t) = \sum_{n=0}^{\infty} \mathbf{J}^{(n)}(\mathbf{r}, t), \quad (5.3)$$

where

$$\mathbf{J}^{(n)}(\mathbf{r}, t) = \frac{1}{(2\pi)^3 n!} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{r}} (\mathbf{q} \cdot \nabla_{\mathbf{q}})^n \mathbf{J}(\mathbf{0}; t) d^3q \quad (5.4)$$

To understand the physics hidden in the various $\mathbf{J}^{(n)}(\mathbf{r}, t)$'s one needs the inverse transformation to the one in (5.1), viz.,

$$\mathbf{J}(\mathbf{q}; t) = \int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) e^{-i\mathbf{q} \cdot \mathbf{r}} d^3r. \quad (5.5)$$

It appears from (5.4) and (5.5) that the term with $n = 0$ is given by

$$\mathbf{J}^{(0)}(\mathbf{r}, t) = \mathbf{J}(\mathbf{0}; t) \delta(\mathbf{r}), \quad (5.6)$$

where $\delta(\mathbf{r})$ is the Dirac delta function, and

$$\mathbf{J}(\mathbf{0}; t) = \int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) d^3r \equiv \mathbf{J}^{\text{ED}}(t) \quad (5.7)$$

is proportional to the spatial mean value of the current density in the (mesoscopic) particle system. As indicated in (5.7) the integral of the current density over the particle domain is called the electric-dipole (ED) current density. The dimension of $\mathbf{J}^{\text{ED}}(t)$ is the same as that of the spatial Fourier transform of the space–time current density $\mathbf{J}(\mathbf{r}, t)$. If only the $n = 0$ term is kept in the moment expansion the mesoscopic (or microscopic) medium behaves like an electric point-dipole, cf. (5.6).

To calculate the term with $n = 1$, namely,

$$\mathbf{J}^{(1)}(\mathbf{r}, t) = (2\pi)^{-3} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{r}} \mathbf{q} \cdot \nabla_{\mathbf{q}} \mathbf{J}(\mathbf{0}; t) d^3q, \quad (5.8)$$

we use that

$$\nabla \delta(\mathbf{r}) = i(2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{q} e^{i\mathbf{q} \cdot \mathbf{r}} d^3q, \quad (5.9)$$

and

$$\nabla_{\mathbf{q}} \mathbf{J}(\mathbf{q}; t) \big|_{\mathbf{q}=\mathbf{0}} = -i \int_{-\infty}^{\infty} \mathbf{r} \mathbf{J}(\mathbf{r}, t) d^3r. \quad (5.10)$$

The last result is obtained by operating on (5.5) with $\nabla_{\mathbf{q}}$. By insertion of (5.9) and (5.10) into (5.8) it appears that

$$\mathbf{J}^{(1)}(\mathbf{r}, t) = -\nabla \delta(\mathbf{r}) \cdot \left[\int_{-\infty}^{\infty} \mathbf{r} \mathbf{J}(\mathbf{r}, t) d^3r \right], \quad (5.11)$$

or equivalently

$$\mathbf{J}^{(1)}(\mathbf{r}, t) = -\mathbf{J}^{\text{MD+EQ}}(t) \cdot \nabla \delta(\mathbf{r}), \quad (5.12)$$

where

$$\mathbf{J}^{\text{MD+EQ}}(t) = \int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) \mathbf{r} d^3r. \quad (5.13)$$

The superscript MD+EQ indicates that the second rank tensor $\mathbf{J}^{\text{MD+EQ}}(t)$ is the sum of magnetic dipole (MD) and electric quadrupole (EQ) contributions. The two contributions are related to the symmetric and antisymmetric parts of the tensorial first-order moment of the current density distribution as follows:

$$\mathbf{J}^{\text{MD+EQ}}(t) = \mathbf{J}^{\text{EQ}}(t) + \mathbf{J}^{\text{MD}}(t), \quad (5.14)$$

where

$$\mathbf{J}^{\text{EQ}}(t) = \frac{1}{2} \int_{-\infty}^{\infty} (\mathbf{J}(\mathbf{r}, t) \mathbf{r} + \mathbf{r} \mathbf{J}(\mathbf{r}, t)) d^3 r, \quad (5.15)$$

and

$$\mathbf{J}^{\text{MD}}(t) = \frac{1}{2} \int_{-\infty}^{\infty} (\mathbf{J}(\mathbf{r}, t) \mathbf{r} - \mathbf{r} \mathbf{J}(\mathbf{r}, t)) d^3 r. \quad (5.16)$$

Following the method outlined above one may show that the general term $\mathbf{J}^{(n)}(\mathbf{r}, t)$ is given by

$$\mathbf{J}^{(n)}(\mathbf{r}, t) = (-1)^n \left[\int_{-\infty}^{\infty} d^3 r \mathbf{J}(\mathbf{r}, t) \{\mathbf{r}\} \cdot \nabla \right]^n \delta(\mathbf{r}) \quad (5.17)$$

in a notation meant to indicate that the tensorial product of the $(n + 1)$ th rank tensor $\int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) \mathbf{r} \mathbf{r} \cdots \mathbf{r} d^3 r$ ($\mathbf{r} \mathbf{r} \cdots \mathbf{r}$ is a string of n $\mathbf{r}$'s) with the n th rank tensor $\nabla \nabla \cdots \nabla \delta(\mathbf{r})$ ($\nabla \nabla \cdots \nabla$ is a string of n ∇ 's) is to be taken. The integral $\int_{-\infty}^{\infty} \mathbf{J}(\mathbf{r}, t) \mathbf{r} \mathbf{r} \cdots \mathbf{r} d^3 r$ is the n th order tensorial moment of the current density distribution.

In the point-particle description, where the current density is given by (2.29), the electric dipole current density equals

$$\mathbf{J}^{\text{ED}}(t) = \frac{d}{dt} \mathbf{p}(t), \quad (5.18)$$

where

$$\mathbf{p}(t) = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha}(t) \quad (5.19)$$

is the instantaneous electric dipole moment of the point-charge distribution. It is easy to prove that $\mathbf{p}(t)$ is independent of the choice of origo for the coordinate system provided the charge system is globally neutral. By insertion of (2.29) into (5.15) it is easy to show that the electric quadrupole tensor $\mathbf{J}^{\text{EQ}}(t)$ is given by

$$\mathbf{J}^{\text{EQ}}(t) = \frac{d}{dt} \mathbf{Q}(t), \quad (5.20)$$

where

$$\mathbf{Q}(t) = \frac{1}{2} \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha}(t) \mathbf{r}_{\alpha}(t) \quad (5.21)$$

is the electric quadrupole moment of the point-charge distribution at time t in the chosen coordinate system. The antisymmetric part of the first-order moment of the current density takes the form

$$\frac{1}{2} \int_{-\infty}^{\infty} (\mathbf{J}(\mathbf{r}, t) \mathbf{r} - \mathbf{r} \mathbf{J}(\mathbf{r}, t)) d^3 r = \frac{1}{2} \sum_{\alpha} q_{\alpha} (\mathbf{v}_{\alpha}(t) \mathbf{r}_{\alpha}(t) - \mathbf{r}_{\alpha}(t) \mathbf{v}_{\alpha}(t)), \quad (5.22)$$

or equivalently

$$\frac{1}{2} \int_{-\infty}^{\infty} (\mathbf{J}(\mathbf{r}, t) \mathbf{r} - \mathbf{r} \mathbf{J}(\mathbf{r}, t)) d^3r = \mathbf{U} \times \sum_{\alpha} \frac{1}{2} q_{\alpha} \mathbf{r}_{\alpha}(t) \times \mathbf{v}_{\alpha}(t). \quad (5.23)$$

In terms of the instantaneous magnetic dipole moment of the point-charge distribution, viz.,

$$\mathbf{m}(t) = \frac{1}{2} \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha}(t) \times \dot{\mathbf{r}}_{\alpha}(t), \quad (5.24)$$

the magnetic dipole tensor $\mathbf{J}^{\text{MD}}(t)$ is given by

$$\mathbf{J}^{\text{MD}}(t) = \mathbf{U} \times \mathbf{m}(t). \quad (5.25)$$

The magnetic dipole moment can also be expressed in terms of the individual relativistic orbital angular momenta

$$\mathbf{L}_{\alpha}(t) = \mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t) \quad (5.26)$$

of the particles. Hence,

$$\mathbf{m}(t) = \sum_{\alpha} \frac{q_{\alpha}}{2m_{\alpha}(v_{\alpha}(t))} \mathbf{L}_{\alpha}(t), \quad (5.27)$$

where $m_{\alpha}(v_{\alpha}(t)) = m_{\alpha}(0)[1 - (v_{\alpha}(t)/c_0)^2]^{-1/2}$ is the relativistic mass of the particle number α at time t .

On the basis of the results in (5.20) and (5.25) it appears that the second rank tensor $\mathbf{J}^{\text{MD+EQ}}(t)$ (5.13), which characterizes the $n = 1$ contribution in the moment expansion of $\mathbf{J}(\mathbf{r}, t)$ (see (5.12)), is given by

$$\mathbf{J}^{\text{EQ+MD}}(t) = \frac{d}{dt} \mathbf{Q}(t) + \mathbf{U} \times \mathbf{m}(t). \quad (5.28)$$

A result formally identical to this plays an important role in the quantum theory of the electrodynamics of mesoscopic (and microscopic) objects.

The electric quadrupole moment often is represented by the continuum expression

$$\mathbf{Q}(t) = \frac{1}{2} \int_{-\infty}^{\infty} \mathbf{r} \mathbf{r} \rho(\mathbf{r}, t) d^3r, \quad (5.29)$$

and the agreement with (5.21) follows readily by insertion of the point-particle charge density in (2.28). The equation of continuity for the charge (2.108) gives

$$\frac{d}{dt} \mathbf{Q}(t) = -\frac{1}{2} \int_{-\infty}^{\infty} \mathbf{r} \mathbf{r} \nabla \cdot \mathbf{J}(\mathbf{r}, t) d^3r, \quad (5.30)$$

and it is easy to show that this expression for $\mathbf{J}^{\text{EQ}}(t)$ (5.20) leads back to (5.15). Partial integrations of (5.30) thus give

$$\frac{d}{dt} \mathbf{Q}(t) = \frac{1}{2} \int_{-\infty}^{\infty} \sum_{i=x,y,z} J_i \frac{\partial}{\partial i} (\mathbf{r} \mathbf{r}) d^3 r, \quad (5.31)$$

under the assumption that the current density distribution is located in a finite region of space so that surface integrals at infinity vanish. Utilizing that

$$\frac{\partial}{\partial i} (\mathbf{r} \mathbf{r}) = \hat{\mathbf{i}} \mathbf{r} + \mathbf{r} \hat{\mathbf{i}}, \quad (5.32)$$

where $\hat{\mathbf{i}}$ is a unit vector along the i th Cartesian axis, the agreement between the formulas in (5.15) and (5.30) follows immediately. In textbooks, the magnetic dipole moment of a continuous current density distribution usually is given by the formula

$$\mathbf{m}(t) = \frac{1}{2} \int_{-\infty}^{\infty} \mathbf{r} \times \mathbf{J}(\mathbf{r}, t) d^3 r. \quad (5.33)$$

Since

$$\mathbf{U} \times (\mathbf{r} \times \mathbf{J}) = \mathbf{J} \mathbf{r} - \mathbf{r} \mathbf{J}, \quad (5.34)$$

it appears that (5.16) and (5.25) are in agreement when $\mathbf{m}(t)$ is given by (5.33). By inserting (2.29) into (5.33) one regains the expression in (5.24) for the magnetic dipole moment of a point-charge distribution.

5.2 Electric and Magnetic Dipole Fields

If a source current density distribution is confined to a sufficiently small region in space, i.e., roughly speaking a region much smaller in linear extension than a typical wavelength of the relevant field, the emitted field can with advantage be calculated on the basis of the moment expansion of the current density. In this section, results are presented for the electromagnetic fields generated by electric and magnetic dipole current densities. For brevity we confine ourselves to a study of the fields in the space–frequency domain.

Let us first consider the fields from the electric dipole current density

$$\mathbf{J}^{(0)}(\mathbf{r}, \omega) = -i\omega \mathbf{p}(\omega) \delta(\mathbf{r}), \quad (5.35)$$

$\mathbf{p}(\omega)$ being the electric dipole moment in the frequency domain. In the Lorenz gauge, the vector potential, $\mathbf{A}^{\text{ED}}(\mathbf{r}; \omega)$, generated by $\mathbf{J}^{(0)}(\mathbf{r}; \omega)$ is readily obtained from (3.10). Hence,

$$\mathbf{A}^{\text{ED}}(\mathbf{r}; \omega) = -i\mu_0 \omega g(\mathbf{r}; \omega) \mathbf{p}(\omega), \quad (5.36)$$

with $g(r, \omega)$ given by (3.13) [$R = r$]. The electric ($\mathbf{E}^{\text{ED}}(\mathbf{r}; \omega)$) and magnetic ($\mathbf{B}^{\text{ED}}(\mathbf{r}; \omega)$) fields from the electric dipole source can also be found immediately from (3.21) and (3.25). Thus,

$$\mathbf{E}^{\text{ED}}(\mathbf{r}; \omega) = \mu_0 \omega^2 \mathbf{G}(\mathbf{r}; \omega) \cdot \mathbf{p}(\omega), \quad (5.37)$$

and

$$\mathbf{B}^{\text{ED}}(\mathbf{r}; \omega) = c_0^{-1} \mu_0 \omega^2 \mathbf{G}_M(\mathbf{r}; \omega) \cdot \mathbf{p}(\omega), \quad (5.38)$$

with $\mathbf{G}(\mathbf{r}; \omega)$ and $\mathbf{G}_M(\mathbf{r}; \omega)$ given by (3.32) and (3.33) [$R=r$]. The result in (5.38) can be reduced to a form commonly found in textbooks noting that

$$\mathbf{U} \times \hat{\mathbf{r}} \cdot \mathbf{p}(\omega) = \hat{\mathbf{r}} \times \mathbf{p}(\omega). \quad (5.39)$$

Let us next consider the fields generated by the magnetic dipole current density

$$\mathbf{J}_{\text{MD}}^{(1)}(\mathbf{r}; \omega) = -\mathbf{U} \times \mathbf{m}(\omega) \cdot \nabla \delta(\mathbf{r}), \quad (5.40)$$

$\mathbf{m}(\omega)$ being the magnetic dipole moment in the frequency domain. The vector potential, $\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega)$, associated to (5.40) is in the Lorenz gauge given by

$$\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega) = -\mu_0 \mathbf{U} \times \mathbf{m}(\omega) \cdot \left[\int_{-\infty}^{\infty} g(R; \omega) \nabla' \delta(\mathbf{r}') d^3 r' \right], \quad (5.41)$$

cf. (3.10). A partial integration in (5.41), and use of the integral property of the delta function, then give

$$\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega) = -\mu_0 \mathbf{U} \times \mathbf{m}(\omega) \cdot \nabla g(r; \omega), \quad (5.42)$$

because $\nabla' g = -\nabla g$, and the quantity $g(R; \omega) \delta(\mathbf{r}')$ vanishes for $\mathbf{r}' \neq \mathbf{0}$ [and thus in the integration limits]. Since $\mathbf{U} \times \mathbf{m}(\omega)$ is an antisymmetric tensor, $\nabla g(r; \omega) = \hat{\mathbf{r}} \partial g(r; \omega) / \partial r$, and $\hat{\mathbf{r}} \cdot \mathbf{U} \times \mathbf{m} = \hat{\mathbf{r}} \times \mathbf{m}$, (5.42) is reduced to

$$\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega) = \mu_0 \frac{\partial g(r; \omega)}{\partial r} \hat{\mathbf{r}} \times \mathbf{m}(\omega), \quad (5.43)$$

or in explicit form

$$\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega) = \mu_0 \frac{e^{iq_0 r}}{4\pi r} \left(i q_0 - \frac{1}{r} \right) \hat{\mathbf{r}} \times \mathbf{m}(\omega). \quad (5.44)$$

The tensor relation $\mathbf{U} \times \hat{\mathbf{r}} \cdot \mathbf{m}(\omega) = \hat{\mathbf{r}} \times \mathbf{m}(\omega)$, together with the expression in (3.33) for $\mathbf{G}_M(\mathbf{R}; \omega)$, show that $\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega)$ also can be written in the form

$$\mathbf{A}^{\text{MD}}(\mathbf{r}; \omega) = \frac{i \mu_0 \omega}{c_0} \mathbf{G}_M(\mathbf{r}; \omega) \cdot \mathbf{m}(\omega). \quad (5.45)$$

If one now compares (5.38) and (5.45), and remember that $\mathbf{B} = \nabla \times \mathbf{A}$, and $\mathbf{E} = (ic_0^2/\omega)\nabla \times \mathbf{B}$ (Maxwell (3.7) in vacuum), the following result is readily obtained for the magnetic field from a magnetic dipole:

$$\mathbf{B}^{\text{MD}}(\mathbf{r}; \omega) = c_0^{-2} \mu_0 \omega^2 \mathbf{G}(\mathbf{r}; \omega) \cdot \mathbf{m}(\omega). \quad (5.46)$$

A glance at (5.37) and (5.46) shows the structural similarity of the magnetic field from a magnetic dipole and the electric field from an electric dipole. The extra factor c_0^{-2} in (5.46) stems from the associations $\epsilon_0 \mathbf{B}^{\text{MD}} \Leftrightarrow \mathbf{E}^{\text{ED}}$ and $c_0^{-1} \mathbf{m}(\omega) \Leftrightarrow \mathbf{p}(\omega)$. The Maxwell equation in (3.7) (with $\mathbf{J} = \mathbf{0}$) and (3.28) finally give us an expression for the electric field from a magnetic dipole, viz.,

$$\mathbf{E}^{\text{MD}}(\mathbf{r}; \omega) = -c_0^{-1} \mu_0 \omega^2 \mathbf{G}_M(\mathbf{r}; \omega) \cdot \mathbf{m}(\omega). \quad (5.47)$$

By means of the dyadic Green functions $\mathbf{G}(\mathbf{r}; \omega)$ and $\mathbf{G}_M(\mathbf{r}; \omega)$ quite simple formulas ((5.37), (5.38), (5.46), and (5.47)) for the electric and magnetic dipole fields have hence been established. The formulas give the relevant fields in the near-, mid-, and far-field zones.

5.3 Electric Quadrupole Fields

To obtain the electric quadrupole contribution to the vector potential in the Lorenz gauge one just needs to replace the magnetic dipole tensor $\mathbf{J}^{\text{MD}}(\omega) = \mathbf{U} \times \mathbf{m}(\omega)$ in (5.42) with the electric quadrupole tensor $\mathbf{J}^{\text{EQ}}(\omega) = -i\omega \mathbf{Q}(\omega)$. Thus,

$$\mathbf{A}^{\text{EQ}}(\mathbf{r}; \omega) = i\mu_0 \omega \mathbf{Q}(\omega) \cdot \nabla g(\mathbf{r}; \omega), \quad (5.48)$$

and then

$$\mathbf{A}^{\text{EQ}}(\mathbf{r}, \omega) = i\mu_0 \omega \frac{e^{iq_0 r}}{4\pi r} \left(iq_0 - \frac{1}{r} \right) \mathbf{Q}(\omega) \cdot \hat{\mathbf{r}}. \quad (5.49)$$

The electric and magnetic fields generated by the electric quadrupole current density

$$\mathbf{J}_{\text{EQ}}^{(1)}(\mathbf{r}; \omega) = i\omega \mathbf{Q}(\omega) \cdot \nabla \delta(\mathbf{r}) \quad (5.50)$$

outside the source may be determined via the general formulas in (3.21) and (3.25). The i th component of the electric field from the electric quadrupole current density distribution hence is given by

$$E_i^{\text{EQ}}(\mathbf{r}; \omega) = -\mu_0 \omega^2 \sum_{j,k} \int_{-\infty}^{\infty} G_{ij}(\mathbf{r} - \mathbf{r}'; \omega) Q_{jk}(\omega) \nabla'_k \delta(\mathbf{r}') d^3 r', \quad (5.51)$$

and a partial integration in combination with the relation $\nabla'_k = -\nabla_k$ and use of the integral property of the Dirac delta function lead to the expression

$$E_i^{\text{EQ}}(\mathbf{r}; \omega) = -\mu_0 \omega^2 \sum_{j,k} \nabla_k G_{ij}(\mathbf{r}; \omega) Q_{jk}(\omega). \quad (5.52)$$

Since the Green tensor is symmetric, (5.52) can be rewritten in the form

$$E_i^{\text{EQ}}(\mathbf{r}; \omega) = -\mu_0 \omega^2 \sum_{j,k} Q_{jk} \nabla_k G_{ji}(\mathbf{r}; \omega). \quad (5.53)$$

Using the abbreviated notation

$$\sum_{j,k} A_{jk} B_k C_{ji} \equiv (\mathbf{A} : \mathbf{B} \mathbf{C})_i, \quad (5.54)$$

the electric field from an electric quadrupole source, thus, is given by

$$\mathbf{E}^{\text{EQ}}(\mathbf{r}; \omega) = -\mu_0 \omega^2 \mathbf{Q}(\omega) : \nabla \mathbf{G}(\mathbf{r}; \omega) \quad (5.55)$$

in the space–frequency domain. To obtain the magnetic field from an electric quadrupole current density source one just needs the replacement $\mathbf{G}(\mathbf{r}; \omega) \Rightarrow c_o^{-1} \mathbf{G}_M(\mathbf{r}; \omega)$ in (5.55), cf. (3.21) and (3.25). In our compact notation, the magnetic field from an electric quadrupole source thus is given by

$$\mathbf{B}^{\text{EQ}}(\mathbf{r}; \omega) = -c_o^{-1} \mu_0 \omega^2 \mathbf{Q}(\omega) : \nabla \mathbf{G}_M(\mathbf{r}; \omega). \quad (5.56)$$

In Cartesian coordinates, the expressions for the third rank tensors $\nabla \mathbf{G}(\mathbf{r}; \omega)$ and $\nabla \mathbf{G}_M(\mathbf{r}; \omega)$ are somewhat complicated, and there is no need to present them here. In spherical coordinates the expressions for these tensors are much simpler because only ∇ -operations on the Huygens propagator are needed. With the unit tensor expressed in terms of the local unit vectors (3.34) one obtains

$$\nabla \mathbf{G}(\mathbf{r}; \omega) = \hat{\mathbf{r}} U \frac{\partial g(r; \omega)}{\partial r} + q_0^{-2} \hat{\mathbf{r}} \hat{\mathbf{r}} \hat{\mathbf{r}} \frac{\partial^3 g(r; \omega)}{\partial r^3}, \quad (5.57)$$

and

$$\nabla \mathbf{G}_M(\mathbf{r}; \omega) = (i q_0)^{-1} \hat{\mathbf{r}} U \times \hat{\mathbf{r}} \frac{\partial^2 g(r; \omega)}{\partial r^2}. \quad (5.58)$$

Before finishing this section let us briefly compare the distance (r) dependences of the various electric and magnetic fields calculated in Sects. 5.2 and 5.3. The dyadic Green function $\mathbf{G}(\mathbf{r}; \omega)$ characterizes the fields $\mathbf{E}^{\text{ED}}(\mathbf{r}; \omega)$ and $\mathbf{B}^{\text{MD}}(\mathbf{r}; \omega)$ from electric and magnetic dipoles, and these fields therefore have terms varying as r^{-1} , r^{-2} , and r^{-3} . The near-field term is missing for the fields $\mathbf{B}^{\text{ED}}(\mathbf{r}; \omega)$ and $\mathbf{E}^{\text{MD}}(\mathbf{r}; \omega)$ because these fields are characterized by the Green function

$\mathbf{G}_M(\mathbf{r}; \omega)$ which only has r^{-1} and r^{-2} terms. The electric and magnetic fields from a quadrupole current density source are characterized by the tensors $\nabla \mathbf{G}(\mathbf{r}; \omega)$ and $\nabla \mathbf{G}_M(\mathbf{r}; \omega)$, respectively, and $\mathbf{E}^{\text{EQ}}(\mathbf{r}; \omega)$ therefore has terms varying as r^{-1} , r^{-2} , r^{-3} , and r^{-4} . A term with a r^{-4} distance dependence is not present in $\mathbf{B}^{\text{EQ}}(\mathbf{r}; \omega)$.

5.4 Transverse Electromagnetic Multipole Waves

After having discussed the electric and magnetic dipole fields (Sect. 5.2) and the electric quadrupole field (Sect. 5.3) from a localized current density distribution we turn to the development of a systematic approach for higher-order multipoles. Here, and in Sect. 5.5, our treatment is limited to transverse (divergence-free) electromagnetic fields, but the theory is formulated in such a manner that longitudinal (rotational-free) multipole fields can be incorporated quite easily if wished. In near-field electrodynamics the interplay between transverse and longitudinal multipole fields is important, not least in the first and second-quantized theories for photons and their generation and destruction in interaction with matter.

5.4.1 Spherical Scalar Waves

As a prelude to the vector spherical multipole problem we consider the Helmholtz equation for the scalar field $V(\mathbf{r}; \omega)$, i.e.,

$$(\nabla^2 + q_0^2)V(\mathbf{r}; \omega) = 0. \quad (5.59)$$

In source-free regions of space, where $\mathbf{J}(\mathbf{r}; \omega) = \mathbf{0}$ and $\rho(\mathbf{r}; \omega) = 0$, the Cartesian components of the vector potential and the scalar potential satisfy this equation in the Lorenz gauge, cf. (2.14), (2.15), and (3.43). Also, the Cartesian components of the electric and magnetic fields obey the Helmholtz equation in empty space, cf. (3.47) (with $\nabla \cdot \mathbf{E}(\mathbf{r}; \omega) = 0$) and (3.50). In preparation for the development of the electromagnetic multipole formalism, one seeks the general solution of (5.59) in spherical coordinates (r, θ, φ) . In these coordinates the Laplace operator is given by

$$\nabla^2 = \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}. \quad (5.60)$$

The separation of the radial (r) and angular (θ, φ) variables leads to the well-known expansion

$$V(\mathbf{r}; \omega) = \sum_{J, M} R_J(r) Y_{JM}(\theta, \varphi), \quad (5.61)$$

where the $Y_{JM}(\theta, \varphi)$'s are the spherical harmonics. The parameter J must be zero or a positive integer and the integer M can take on only the values $-J, -J + 1, \dots, 0, \dots, J - 1, J$. The dependence of the various spherical harmonics on the polar angle (θ) is given by the associated Legendre functions $P_J^M(\cos \theta)$, and the azimuth angle (φ) dependence by $\exp(iM\varphi)$. Thus,

$$Y_{JM}(\theta, \varphi) = \sqrt{\frac{2J+1}{4\pi} \frac{(J-M)!}{(J+M)!}} P_J^M(\cos \theta) e^{iM\varphi}. \quad (5.62)$$

The spherical harmonics in (5.62) form a complete orthogonal set of functions on the surface of the unit sphere. The orthonormality condition is

$$\int_0^{2\pi} \int_0^\pi Y_{J'M'}^*(\theta, \varphi) Y_{JM}(\theta, \varphi) \sin \theta \, d\theta \, d\varphi = \delta_{JJ'} \delta_{MM'}, \quad (5.63)$$

and the completeness is expressed via the relation

$$\sum_{J=0}^{\infty} \sum_{M=-J}^J Y_{JM}^*(\theta', \varphi') Y_{JM}(\theta, \varphi) = \delta(\varphi - \varphi') \delta(\cos \theta - \cos \theta'). \quad (5.64)$$

The spherical harmonics satisfy the partial differential equation

$$-\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] Y_{JM}(\theta, \varphi) = J(J+1) Y_{JM}(\theta, \varphi). \quad (5.65)$$

The radial functions satisfy the M -independent ordinary differential equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + q_0^2 - \frac{J(J+1)}{r^2} \right] R_J(r) = 0. \quad (5.66)$$

With the substitution

$$R_J(r) = \frac{1}{r^{1/2}} u_J(r), \quad (5.67)$$

Equation (5.66) is transformed into a Bessel equation of half-integer order $\nu = J + \frac{1}{2}$ for $u_J(r)$, viz.,

$$\left[\frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + q_0^2 - \frac{(J + \frac{1}{2})^2}{r^2} \right] u_J(r) = 0. \quad (5.68)$$

Since the Bessel function of the first kind, and order $\nu = J + \frac{1}{2}$, $J_{J+\frac{1}{2}}(q_0 r)$, and the Neumann function (Bessel function of the second kind) of order $\nu = J + \frac{1}{2}$, $N_{J+\frac{1}{2}}(q_0 r)$, are linearly independent solutions to (5.68), the general solution to the radial equation in (5.66) is

$$R_J(r) = \frac{A_J}{r^{\frac{1}{2}}} J_{J+\frac{1}{2}}(q_0 r) + \frac{B_J}{r^{\frac{1}{2}}} N_{J+\frac{1}{2}}(q_0 r), \quad (5.69)$$

where the constants A_J and B_J will be determined by the boundary conditions. It is customary to define spherical Bessel ($j_J(x)$) and Neumann ($n_J(x)$) functions as follows:

$$j_J(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} J_{J+\frac{1}{2}}(x), \quad (5.70)$$

$$n_J(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} N_{J+\frac{1}{2}}(x), \quad (5.71)$$

and write the general solution to the radial equation in terms of these. Instead one may express $R_J(r)$ with the help of the spherical Hankel functions of the first and second kind and order J . These are denoted by $h_J^{(1)}(x)$ and $h_J^{(2)}(x)$, respectively, and they are defined by

$$h_J^{(1)}(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} \left[J_{J+\frac{1}{2}}(x) + i N_{J+\frac{1}{2}}(x) \right], \quad (5.72)$$

$$h_J^{(2)}(x) = \left(\frac{\pi}{2x}\right)^{\frac{1}{2}} \left[J_{J+\frac{1}{2}}(x) - i N_{J+\frac{1}{2}}(x) \right]. \quad (5.73)$$

For real x , $h_J^{(2)}(x)$ is the complex conjugate of $h_J^{(1)}(x)$. The spherical Hankel functions are particularly useful in studies of radiation problems because they relate to propagating fields. The general solution to the Helmholtz equation in spherical coordinates can finally be written

$$V(\mathbf{r}; \omega) = \sum_{J,M} \left[A_{JM}^{(1)} h_J^{(1)}(q_0 r) + A_{JM}^{(2)} h_J^{(2)}(q_0 r) \right] Y_{JM}(\theta, \varphi), \quad (5.74)$$

where $A_{JM}^{(1)}$ and $A_{JM}^{(2)}$ are arbitrary constants.

5.4.2 Interlude: Angular Field Momentum Operator $\hat{\mathbf{J}}$

Let us make a brief pause in the development of the formalism for electromagnetic multipole waves and in the view of quantum mechanics take a brief look at the angular functions and the differential equation they satisfy. An equation formally identical to (5.65) appears in the elementary quantum mechanics of massive particles [164]. Here, it is written in the form

$$\hat{\mathbf{J}}^2 Y_{JM} = J(J+1) Y_{JM}, \quad (5.75)$$

where

$$\hat{\mathbf{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \quad (5.76)$$

is the square of the dimensionless orbital angular momentum operator

$$\hat{\mathbf{J}} = \frac{1}{i} \mathbf{r} \times \nabla. \quad (5.77)$$

If $\hbar = h/(2\pi)$, where h is Planck's constant, $\hbar \hat{\mathbf{J}}$ is precisely the orbital angular momentum operator of a particle with position operator $\hat{\mathbf{r}} = \mathbf{r}$ and momentum operator $\hat{\mathbf{p}} = (\hbar/i)\nabla$. Although it is custom to denote the orbital angular momentum operator of a (massive) particle by $\hat{\mathbf{L}}$ we have used the symbol $\hat{\mathbf{J}}$ above. The reason for this appears when the physics in the Maxwell theory for free space is given a quantum mechanical interpretation. The “classical” theory then turns into a wave mechanical (first-quantized) theory for the photon, the elementary particle associated to the free electromagnetic field. The $\hat{\mathbf{J}}$ -operator now becomes the *total* angular momentum operator for the photon. Conceptually, it is useful to divide the $\hat{\mathbf{J}}$ -operator into a sum of two parts, i.e., $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$, where $\hat{\mathbf{L}}$ is the *orbital* angular momentum of the photon (around a chosen reference point in space), and $\hat{\mathbf{S}}$ is the intrinsic angular momentum (spin) operator of the photon. The first-quantized theory of the photon, including the angular momentum formalism of this massless particle, is developed and discussed in some detail in Part II of this book (see, in particular, Chaps. 15–17).

The (dimensionless) angular-momentum operator for the electromagnetic field satisfies the vectorial commutator rule

$$\hat{\mathbf{J}} \times \hat{\mathbf{J}} = i \hat{\mathbf{J}}. \quad (5.78)$$

In a broader context, only operators $\hat{\mathbf{O}}$ which fulfil the dimensionless commutator relation $\hat{\mathbf{O}} \times \hat{\mathbf{O}} = i \hat{\mathbf{O}}$ qualify as angular momentum operators in quantum theory. Instead of using the components $\hat{J}_x$ and $\hat{J}_y$ it is often more convenient to introduce the linear combinations [164]

$$\hat{J}_+ = \hat{J}_x + i \hat{J}_y, \quad (5.79)$$

$$\hat{J}_- = \hat{J}_x - i \hat{J}_y. \quad (5.80)$$

The operators $\hat{J}_+$ and $\hat{J}_-$ are not Hermitian, but they are adjoints of each other. By means of $\hat{J}_+$ and $\hat{J}_-$ one can establish the following recursion relations for the spherical harmonics of a given quantum number J [164]:

$$\hat{J}_+ Y_{JM} = \sqrt{(J-M)(J+M+1)} Y_{J, M+1}, \quad (5.81)$$

$$\hat{J}_- Y_{JM} = \sqrt{(J+M)(J-M+1)} Y_{J, M-1}. \quad (5.82)$$

We shall make use of (5.81) and (5.82) in the next subsection.

5.4.3 Electric and Magnetic Multipole Fields

Let us now return to the development of the multipole expansion for the electromagnetic field in source-free regions of space. The establishment of the standard theory described here follows a path suggested by Bouwkamp and Casimir [115]. Later in the book I shall describe another multipole expansion scheme which relates more directly to the wave mechanics of transverse, longitudinal and scalar photons.

In a source-free region of space it follows from the Maxwell equations that the electric and magnetic fields satisfy the Helmholtz equation, i.e.,

$$(\nabla^2 + q_0^2) \mathbf{E}(\mathbf{r}; \omega) = \mathbf{0}, \quad (5.83)$$

$$(\nabla^2 + q_0^2) \mathbf{B}(\mathbf{r}; \omega) = \mathbf{0}, \quad (5.84)$$

and that both the electric and magnetic fields are divergence-free, $\nabla \cdot \mathbf{E}(\mathbf{r}; \omega) = \nabla \cdot \mathbf{B}(\mathbf{r}; \omega) = 0$. By scalar multiplication of (5.83) and (5.84) with $\mathbf{r}$, and by use of the general relation

$$\mathbf{r} \cdot \nabla^2 \mathbf{V} = \nabla^2(\mathbf{r} \cdot \mathbf{V}) - 2\nabla \cdot \mathbf{V}, \quad (5.85)$$

it readily appears that the scalars $\mathbf{r} \cdot \mathbf{E}(\mathbf{r}; \omega)$ and $\mathbf{r} \cdot \mathbf{B}(\mathbf{r}; \omega)$ both satisfy the Helmholtz equation:

$$(\nabla^2 + q_0^2)(\mathbf{r} \cdot \mathbf{E}(\mathbf{r}; \omega)) = 0, \quad (5.86)$$

$$(\nabla^2 + q_0^2)(\mathbf{r} \cdot \mathbf{B}(\mathbf{r}; \omega)) = 0. \quad (5.87)$$

The general solution for these scalar equations thus may be given by expressions of the form in (5.74).

One now defines a magnetic multipole field (superscript (M)) of order (J, M) by the conditions

$$\mathbf{r} \cdot \mathbf{B}_{JM}^{(M)} = \frac{\mu_0}{q_0} J(J+1) g_J(q_0 r) Y_{JM}(\theta, \varphi), \quad (5.88)$$

$$\mathbf{r} \cdot \mathbf{E}_{JM}^{(M)} = 0, \quad (5.89)$$

where $g_J(q_0 r)$ has the general form $g_J(q_0 r) = A_J^{(1)} h_J^{(1)}(q_0 r) + A_J^{(2)} h_J^{(2)}(q_0 r)$, cf. (5.74). From the Maxwell equation in (3.5) one can relate $\mathbf{r} \cdot \mathbf{B}_{JM}^{(M)}$ to $\hat{\mathbf{J}} \cdot \mathbf{E}_{JM}^{(M)}$. Thus

$$\mathbf{r} \cdot \mathbf{B}_{JM}^{(M)} = \frac{1}{i\omega} \mathbf{r} \cdot \nabla \times \mathbf{E}_{JM}^{(M)} = \frac{1}{\omega} \frac{1}{i} \mathbf{r} \times \nabla \cdot \mathbf{E}_{JM}^{(M)} = \frac{1}{\omega} \hat{\mathbf{J}} \cdot \mathbf{E}_{JM}^{(M)}. \quad (5.90)$$

To determine $\mathbf{E}_{JM}^{(M)}$ from (5.88) and (5.90), we first observe that $\mathbf{E}_{JM}^{(M)}$ must have the radial dependence $g_J(q_0 r)$ since the operator $\hat{\mathbf{J}}$ acts only on the angular variables. The angular dependence of $\mathbf{E}_{JM}^{(M)}$ cannot be given by $Y_{JM}(\theta, \varphi)$ because the actions of $\hat{J}_x = (\hat{J}_+ + \hat{J}_-)/2$ and $\hat{J}_y = (\hat{J}_+ - \hat{J}_-)/(2i)$ on $E_{JM,x}^{(M)}$ and $E_{JM,y}^{(M)}$ according to (5.81) and (5.82) will result in combinations of Y_{JM+1} and Y_{JM-1} . To yield

a single Y_{JM} , as required by (5.88) and (5.90), we therefore must have $\mathbf{E}_{JM}^{(M)} = \alpha g_J(q_0 r) \hat{\mathbf{J}} Y_{JM}$, where α is a constant. Using (5.75) we now get $\hat{\mathbf{J}} \cdot \mathbf{E}_{JM}^{(M)} = \alpha g_J J(J+1) Y_{JM}$. When this expression is inserted into (5.90) and a comparison is made to (5.88), one finds that the constant α is given by $\alpha = Z_0$, where

$$Z_0 = c_0 \mu_0 = \left(\frac{\mu_0}{\epsilon_0} \right)^{\frac{1}{2}} \quad (5.91)$$

is the impedance of free space. Altogether, the electric and magnetic components of the magnetic multipole field of order (J, M) are

$$\mathbf{E}_{JM}^{(M)}(r, \theta, \varphi) = c_0 \mu_0 g_J(q_0 r) \hat{\mathbf{J}} Y_{JM}(\theta, \varphi), \quad (5.92)$$

$$\mathbf{B}_{JM}^{(M)}(r, \theta, \varphi) = \frac{1}{i\omega} \nabla \times \mathbf{E}_{JM}^{(M)}(r, \theta, \varphi). \quad (5.93)$$

The divergence-free electric field associated with a given magnetic multipole is transverse to the radius vector ($\mathbf{r}$) everywhere in source-free regions of space; see (5.89). Later on in this book we study the magnetic multipole fields associated to the photon field variables, and for these it appears that the *divergence-free electric vector field* is *not* in the geometrical sense transverse to the radius vector in the near- and mid-field zones of a photon source.

The fields of an electric multipole field (superscript (E)) of order (J, M) are specified by the conditions

$$\mathbf{r} \cdot \mathbf{E}_{JM}^{(E)} = -\frac{c_0 \mu_0}{q_0} J(J+1) f_J(q_0 r) Y_{JM}(\theta, \varphi), \quad (5.94)$$

$$\mathbf{r} \cdot \mathbf{B}_{JM}^{(E)} = 0, \quad (5.95)$$

where the radial function $f_J(q_0 r)$ is given by an expression like the one for $g_J(q_0 r)$; see the line below (5.89).

The magnetic field $\mathbf{B}_{JM}^{(E)}$ is everywhere in vacuum transverse to the radius vector, $\mathbf{r}$. Following the procedure used above for the magnetic multipole field it is easy to show that the magnetic and electric parts of the electric multipole field of order (J, M) are

$$\mathbf{B}_{JM}^{(E)}(r, \theta, \varphi) = \mu_0 f_J(q_0 r) \hat{\mathbf{J}} Y_{JM}(\theta, \varphi), \quad (5.96)$$

$$\mathbf{E}_{JM}^{(E)}(r, \theta, \varphi) = \frac{ic_0^2}{\omega} \nabla \times \mathbf{B}_{JM}^{(E)}(r, \theta, \varphi). \quad (5.97)$$

The vector spherical harmonics, $\hat{\mathbf{J}} Y_{JM}$, play as we have seen an important role in the theory of multipole fields, and it is convenient to introduce the normalized form

$$\mathbf{X}_{JM}(\theta, \varphi) = \frac{1}{\sqrt{J(J+1)}} \hat{\mathbf{J}} Y_{JM}(\theta, \varphi), \quad J \neq 0 \quad (5.98)$$

and define $X_{JM}(\theta, \varphi)$ to be identically zero for $J = 0$. Since $Y_{00} = (4\pi)^{-1/2}$ there are no *electrodynamical* fields associated to $(J, M) = (0, 0)$. One can show that the $X_{JM}(\theta, \varphi)$'s satisfy the orthonormality condition

$$\int X_{J'M'}^*(\theta, \varphi) \cdot X_{JM}(\theta, \varphi) d\Omega = \delta_{JJ'} \delta_{MM'}, \quad (5.99)$$

where $d\Omega = \sin \theta d\theta d\varphi$, and the integration extends over the entire angle 4π . For all J, J', M, M' one also has

$$\int X_{J'M'}^*(\theta, \varphi) \cdot \mathbf{r} \times X_{JM}(\theta, \varphi) d\Omega = 0. \quad (5.100)$$

It can be shown that the two set of multipole fields in (5.92), (5.93), (5.96) and (5.97) form a complete set of solutions to the Maxwell equations in a source-free region. By combining the two types of fields one may write the general solution to the free-space Maxwell equations as follows [19]:

$$\begin{aligned} \mathbf{E}(r, \theta, \varphi) = Z_0 \sum_{J,M} \left[\frac{i}{q_0} a_E(J, M) \nabla \times (f_J(q_0 r) X_{JM}(\theta, \varphi)) \right. \\ \left. + Z_0 a_M(J, M) g_J(q_0 r) X_{JM}(\theta, \varphi) \right], \end{aligned} \quad (5.101)$$

$$\begin{aligned} \mathbf{B}(r, \theta, \varphi) = \mu_0 \sum_{J,M} \left[a_E(J, M) f_J(q_0 r) X_{JM}(\theta, \varphi) \right. \\ \left. - \frac{i}{q_0} a_M(J, M) \nabla \times (g_J(q_0 r) X_{JM}(\theta, \varphi)) \right]. \end{aligned} \quad (5.102)$$

The so-called electric and magnetic multipole coefficients $a_E(J, M)$ and $a_M(J, M)$, and the relevant linear combinations of $h_J^{(1)}(q_0 r)$ and $h_J^{(2)}(q_0 r)$ to appear in the functions $f_J(q_0 r)$ and $g_J(q_0 r)$, are determined from the current density distribution of the sources, and the boundary conditions for the fields.

5.5 Microscopic Sources of Multipole Fields

5.5.1 Microscopic Maxwell Equations with a New Electric-Field Variable

The electric and magnetic multipole fields studied in Sect. 5.4 are all divergence-free both with regard to their electric and magnetic field parts, i.e., $\nabla \cdot \mathbf{E}_{JM}^{(E)} = \nabla \cdot \mathbf{E}_{JM}^{(M)} = \nabla \cdot \mathbf{B}_{JM}^{(E)} = \nabla \cdot \mathbf{B}_{JM}^{(M)} = 0$. This of course follows from the fact that

the individual multipole fields are solutions to the Maxwell equations in source-free regions. To examine the connection of the multipole fields with the sources that generate them we start from the microscopic Maxwell–Lorentz equations in the space–frequency domain. Instead of using (3.5)–(3.8) as they stand, it is convenient to introduce a new “electric-field” variable

$$\mathcal{E}(\mathbf{r}; \omega) = \mathbf{E}(\mathbf{r}; \omega) + \frac{i}{\epsilon_0 \omega} \mathbf{J}(\mathbf{r}; \omega). \quad (5.103)$$

The new field $\mathcal{E}$ is divergence-free *everywhere* in space, i.e.,

$$\nabla \cdot \mathcal{E}(\mathbf{r}; \omega) = 0, \quad (5.104)$$

as one readily shows with the help of the Maxwell equation in (3.7) and the equation of continuity (3.15). In source-free regions of space, $\mathcal{E}$ reduces to $\mathbf{E}$. If matter is assumed to consist of point-particles we already in the classical theory only deals with fields outside the actual positions of these particles. In quantum mechanics the current density distribution forms a continuum in space in the quantum statistical sense. In the quantum theory, $\mathcal{E}$ and $\mathbf{E}$ will be different inside the quantum statistical $\mathbf{J}(\mathbf{r}; \omega)$ -distribution. The price we have paid in order to introduce a divergence-free “electric-field” variable is that we have mixed $\mathbf{E}$ and $\mathbf{J}$ in the source region. It is possible to avoid this mixing by a rigorous and unique (up to a constant) division of the original electric field, $\mathbf{E}(\mathbf{r}; \omega)$, into its divergence-free ($\mathbf{E}_T$) and rotational-free ($\mathbf{E}_L$) vector parts, $\mathbf{E} = \mathbf{E}_T + \mathbf{E}_L$. The T–L division is extremely convenient for quantum studies in near-field electrodynamics as we shall realize in Parts II and III. In terms of the fields $\mathcal{E}(\mathbf{r}; \omega)$ and $\mathbf{B}(\mathbf{r}; \omega)$ the microscopic Maxwell–Lorentz equations given in (3.5)–(3.8) read

$$\nabla \times \mathcal{E}(\mathbf{r}; \omega) = \frac{i}{\epsilon_0 \omega} \mathbf{J}(\mathbf{r}; \omega) + i \omega \mathbf{B}(\mathbf{r}; \omega), \quad (5.105)$$

$$\nabla \cdot \mathcal{E}(\mathbf{r}; \omega) = 0, \quad (5.106)$$

$$\nabla \times \mathbf{B}(\mathbf{r}; \omega) = -\frac{i \omega}{c_0^2} \mathcal{E}(\mathbf{r}; \omega), \quad (5.107)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}; \omega) = 0. \quad (5.108)$$

The two curl equations can be combined in the usual manner, and upon use of the fact that $\mathcal{E}(\mathbf{r}; \omega)$ and $\mathbf{B}(\mathbf{r}; \omega)$ are divergence-free, one arrives at the inhomogeneous microscopic Helmholtz equations

$$(\nabla^2 + q_0^2) \mathcal{E}(\mathbf{r}; \omega) = \frac{1}{i \epsilon_0 \omega} \nabla \times (\nabla \times \mathbf{J}(\mathbf{r}; \omega)), \quad (5.109)$$

$$(\nabla^2 + q_0^2) \mathbf{B}(\mathbf{r}; \omega) = -\mu_0 \nabla \times \mathbf{J}(\mathbf{r}; \omega). \quad (5.110)$$

5.5.2 Interlude: Spherical Wave Expansion of the Huygens Propagator

To determine the multipole coefficients $a_E(J, M)$ and $a_M(J, M)$ associated with the source distribution given in (5.109) and (5.110), we make use of the spherical wave expansion of the outgoing scalar propagator $g(|\mathbf{r} - \mathbf{r}'|; \omega) = \exp(iq_0|\mathbf{r} - \mathbf{r}'|)/(4\pi|\mathbf{r} - \mathbf{r}'|)$. Since the propagator for $\mathbf{r} \neq \mathbf{r}'$ satisfies the homogeneous Helmholtz equation, see (3.42), and is symmetric in the source ($\mathbf{r}'$) and observation ($\mathbf{r}$) coordinates, $g(|\mathbf{r} - \mathbf{r}'|; \omega)$ will be given by an expansion of the form

$$g(|\mathbf{r} - \mathbf{r}'|; \omega) = \sum_{J,M} R_J(r, r') Y_{JM}^*(\theta', \varphi') Y_{JM}(\theta, \varphi), \quad (5.111)$$

cf. (5.59) and (5.61). In spherical coordinates the Dirac delta function is given by

$$\delta(\mathbf{r} - \mathbf{r}') = |\mathcal{Y}|^{-1} \delta(r - r') \delta(\theta - \theta') \delta(\varphi - \varphi'), \quad (5.112)$$

where $\mathcal{Y} = r^2 \sin \theta$ is the Jacobian of the transformation $(x, y, z) \Rightarrow (r, \theta, \varphi)$. With the help of the rule [165]

$$\delta(f(x)) = \sum_i \frac{1}{\left| \frac{df}{dx}(x_i) \right|} \delta(x - x_i), \quad (5.113)$$

valid when $f(x)$ is assumed to have only simple zeros, located at $x = x_i$, one gets

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{r^2} \delta(r - r') \delta(\cos \theta - \cos \theta') \delta(\varphi - \varphi'). \quad (5.114)$$

The completeness relation in (5.64) finally allows one to write $\delta(\mathbf{r} - \mathbf{r}')$ as follows:

$$\delta(\mathbf{r} - \mathbf{r}') = \frac{1}{r^2} \delta(r - r') \sum_{J,M} Y_{JM}^*(\theta', \varphi') Y_{JM}(\theta, \varphi). \quad (5.115)$$

When (5.111) and (5.115) are substituted into (3.42) one is lead to the equation

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + q_0^2 - \frac{J(J+1)}{r^2} \right] R_J(r, r') = -\frac{1}{r^2} \delta(r - r') \quad (5.116)$$

for $R_J(r, r')$. If we denote by $r_{<}$ ($r_{>}$) the smaller (larger) of $|\mathbf{r}|$ and $|\mathbf{r}'|$, the solution that satisfies the boundary conditions of (1) finiteness at the origin, and (2) outgoing waves at infinity is, cf. (5.74),

$$R_J(r, r') = A j_J(q_0 r_{<}) h_J^{(1)}(q_0 r_{>}), \quad (5.117)$$

where $j_J(q_0 r_<) = \frac{1}{2}(h_J^{(1)}(q_0 r_<) + h_J^{(2)}(q_0 r_<))$. Since $d^2/dr^2 + (2/r)d/dr = r^{-1}d^2/dr^2(r)$ it appears upon integration of (5.116) from $r = r' - \epsilon$ to $r = r' + \epsilon$, where ϵ is a positive infinitesimal number that

$$\left\{ \frac{d}{dr}(rR_J) \right\}_{r=r'+\epsilon} - \left\{ \frac{d}{dr}(rR_J) \right\}_{r=r'-\epsilon} = -\frac{1}{r}. \quad (5.118)$$

The function $R_J(r, r')$ thus has a discontinuity in slope at $r = r'$, and this determines the constant A in (5.117). We can also determine A from the relation

$$\frac{e^{iq_0|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} = A \sum_{J,M} \left[h_J^{(1)}(q_0 r_>) Y_{JM}(\hat{\mathbf{r}}_>) \right] \left[j_J(q_0 r_<) Y_{JM}^*(\hat{\mathbf{r}}_<) \right] \quad (5.119)$$

by asymptotic considerations. Thus, for $r_< \rightarrow 0$, one has $j_J(q_0 r_<) \rightarrow 0 = \delta_{J0}$, and since $Y_{00} = (4\pi)^{-1/2}$, we get

$$\frac{e^{iq_0 r_>}}{4\pi r_>} = \frac{A}{4\pi} h_0^{(1)}(q_0 r_>) = \frac{A}{4\pi} \frac{e^{iq_0 r_>}}{i q_0 r_>}, \quad (5.120)$$

and hence $A = i q_0$. For observations points ($\mathbf{r}$) outside a spherical surface completely enclosing the source points ($\mathbf{r}'$) one has $r = r_>$ and $r' = r_<$. In this case, the spherical wave takes the form

$$g(|\mathbf{r} - \mathbf{r}'|; \omega) = i q_0 \sum_{J=0}^{\infty} j_J(q_0 r') h_J^{(1)}(q_0 r) \sum_{M=-J}^J Y_{JM}^*(\theta', \varphi') Y_{JM}(\theta, \varphi). \quad (5.121)$$

We shall make use of this expansion in the next subsection. For quantum mechanical studies of the self-consistent integral equation for the microscopic electric field of a small object the spherical wave expansion may be useful. In this case we shall need the general formula in (5.119) (with $A = i q_0$), since also $\mathbf{r}$ -points inside the domain of the so-called transverse current density distribution play a role in the photon generation process.

5.5.3 Multipole Coefficients

In (5.101) and (5.102), the general solution to the free-space Maxwell equations is written as a superposition of electric and magnetic multipole fields. The strengths of the various multipole fields are expressed in terms of the electric and magnetic multipole coefficients $a_E(J, M)$ and $a_M(J, M)$. A knowledge of the two scalars $\mathbf{r} \cdot \mathbf{E}$ and $\mathbf{r} \cdot \mathbf{B}$ is sufficient to determine these coefficients. Since (1) $\mathbf{r} \cdot \mathbf{X}_{JM} = 0$, because $\mathbf{r} \cdot \hat{\mathbf{J}} = 0$, and (2) $i^{-1} \mathbf{r} \cdot \nabla \times (f_J \mathbf{X}_{JM}) = \hat{\mathbf{J}} \cdot (f_J \mathbf{X}_{JM}) = f_J \hat{\mathbf{J}} \cdot \mathbf{X}_{JM}$,

because the angular momentum operator only acts on the angular variables, and (3) $\hat{\mathbf{J}} \cdot \mathbf{X}_{JM} = [J(J+1)]^{1/2} Y_{JM}$ (use (5.75) and (5.98)), one obtains

$$\mathbf{r} \cdot \mathbf{E} = -\frac{Z_0}{q_0} \sum_{J,M} a_E(J, M) \sqrt{J(J+1)} f_J(q_0 r) Y_{JM}(\theta, \varphi). \quad (5.122)$$

A similar calculation gives

$$\mathbf{r} \cdot \mathbf{B} = \frac{\mu_0}{q_0} \sum_{J,M} a_M(J, M) \sqrt{J(J+1)} g_J(q_0 r) Y_{JM}(\theta, \varphi). \quad (5.123)$$

Utilizing the orthonormality of the spherical harmonics (5.63), we get the following expression for the multipole coefficients (times the associated radial function):

$$f_J(q_0 r) a_E(J, M) = -\frac{q_0}{Z_0} [J(J+1)]^{-\frac{1}{2}} \int_{4\pi} Y_{JM}^* \mathbf{r} \cdot \mathbf{E} \, d\Omega, \quad (5.124)$$

$$g_J(q_0 r) a_M(J, M) = \frac{q_0}{\mu_0} [J(J+1)]^{-\frac{1}{2}} \int_{4\pi} Y_{JM}^* \mathbf{r} \cdot \mathbf{B} \, d\Omega. \quad (5.125)$$

Ultimately, the multipole coefficients are determined by the current density distribution in the source, and (here) the requirement of outgoing waves at infinity. We must, therefore, seek to relate the source currents to the scalars $\mathbf{r} \cdot \mathbf{E}$ and $\mathbf{r} \cdot \mathbf{B}$. Using (5.58), (5.106), and (5.108), one obtains from (5.109) and (5.110)

$$(\nabla^2 + q_0)(\mathbf{r} \cdot \mathbf{E}) = (\epsilon_0 \omega)^{-1} \hat{\mathbf{J}} \cdot (\nabla \times \mathbf{J}(\mathbf{r}; \omega)), \quad (5.126)$$

$$(\nabla^2 + q_0)(\mathbf{r} \cdot \mathbf{B}) = -i\mu_0 \hat{\mathbf{J}} \cdot \mathbf{J}(\mathbf{r}; \omega), \quad (5.127)$$

since $i^{-1} \mathbf{r} \cdot \nabla \times \mathbf{V} = i^{-1} \mathbf{r} \times \nabla \cdot \mathbf{V} = \hat{\mathbf{J}} \cdot \mathbf{V}$, $\mathbf{V} = \nabla \times \mathbf{J}$ (5.126) and $\mathbf{V} = \mathbf{J}$ (5.127). In accordance with the notation used previously in this book, in the formulas above $\hat{\mathbf{J}}$ is the angular-momentum operator of the field, and $\mathbf{J}(\mathbf{r}; \omega)$ is the charge current density of the source. The solutions to the inhomogeneous Helmholtz equations in (5.126) and (5.127) are given by

$$\mathbf{r} \cdot \mathbf{E}(\mathbf{r}; \omega) = -(\epsilon_0 \omega)^{-1} \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \hat{\mathbf{J}}(\theta', \varphi') \cdot (\nabla' \times \mathbf{J}(\mathbf{r}'; \omega)) \, d^3 r', \quad (5.128)$$

and

$$\mathbf{r} \cdot \mathbf{B}(\mathbf{r}; \omega) = i\mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \hat{\mathbf{J}}(\theta', \varphi') \cdot \mathbf{J}(\mathbf{r}'; \omega) \, d^3 r', \quad (5.129)$$

since outgoing waves are required at infinity. The spherical wave expansion of the Huygens propagator, given in (5.121), shows that one must necessarily make the choices $f_J(q_0 r) = g_J(q_0 r) = h_J^{(1)}(q_0 r)$ in (5.122) and (5.123). With the help of the orthonormality condition for the spherical harmonics (5.63), a combination

of (5.121), (5.124), and (5.128) finally results in the following expression for the electric multipole coefficients for the parameter values J and M :

$$a_E(J, M) = \frac{iq_0}{\sqrt{J(J+1)}} \int_{-\infty}^{\infty} j_J(q_0 r) Y_{JM}^*(\theta, \varphi) \hat{\mathbf{J}}(\theta, \varphi) \cdot \nabla \times \mathbf{J}(r, \theta, \varphi; \omega) d^3r. \quad (5.130)$$

From (5.121), (5.125), and (5.129) one obtains for the magnetic multipole coefficient belonging to J and M the expression

$$a_M(J, M) = -\frac{q_0^2}{\sqrt{J(J+1)}} \int_{-\infty}^{\infty} j_J(q_0 r) Y_{JM}(\theta, \varphi) \hat{\mathbf{J}}(\theta, \varphi) \cdot \mathbf{J}(r, \theta, \varphi; \omega) d^3r. \quad (5.131)$$

For a source of *arbitrary* size characterized by the microscopic current density distribution $\mathbf{J}(\mathbf{r}; \omega)$ we have thus obtained the required multipole expansion of the emitted electromagnetic field ((5.101) and (5.102) for $f_J = g_J = h_J^{(1)}$, and with $a_E(J, M)$ and $a_M(J, M)$ given by (5.130) and (5.131)). The expansion holds *everywhere* in space outside the source, and hence also in the so-called rim zone of matter. The rim zone concept will be defined in Sect. 9.2.2.

5.6 Mesoscopic Particle in a Prescribed External Electromagnetic Field

5.6.1 Rate of Energy Transfer

In Sect. 2.6.1, it was realized that the work carried out per unit time by a microscopic electric field $\mathbf{E}(\mathbf{r}, t)$ on a system of charged point-particles characterized by a current density distribution $\mathbf{J}(\mathbf{r}, t)$ was given by $\int_{-\infty}^{\infty} \mathbf{J} \cdot \mathbf{E} d^3r$. Let us assume that we subject the charge distribution to an externally applied field $\mathbf{E}_{\text{ext}}(\mathbf{r}, t)$. The microscopic electric field then consists of the sum of two parts, viz., the external field and the field $\mathbf{E}_{\text{par}}(\mathbf{r}, t)$ generated by the particles themselves:

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_{\text{ext}}(\mathbf{r}, t) + \mathbf{E}_{\text{par}}(\mathbf{r}, t). \quad (5.132)$$

A part of $\mathbf{E}_{\text{par}}(\mathbf{r}, t)$ will arise as a consequence of the motion induced in the particle system by the external field, and the particle dynamics will evolve under the simultaneous action of $\mathbf{E}_{\text{ext}}$ and $\mathbf{E}_{\text{par}}$. If the reaction of the field from the particle system back on the source particles generating the external field is negligible $\mathbf{E}_{\text{ext}}(\mathbf{r}, t)$ can often be considered as a prescribed quantity. The rate of energy transfer to the particle system from the external field is given by $\int_{-\infty}^{\infty} \mathbf{J} \cdot \mathbf{E}_{\text{ext}} d^3r$, and this expression also holds in the continuum description of matter.

If the current density distribution is confined to such a small region of space that the external field varies only slightly across the distribution, the moment expansion scheme for the current density can be used to simplify the expression for the rate of

energy transfer from $\mathbf{E}_{\text{ext}}$. In near-field optics, the moment expansion is often used in studies of the dynamics of atoms, molecules, and mesoscopic particles (quantum dots, wires, etc.). As before, we place the origo of our coordinate system at the center of the charge distribution, and then we make a Taylor series expansion of the external electric field around $\mathbf{r} = \mathbf{0}$, i.e.,

$$\mathbf{E}_{\text{ext}}(\mathbf{r}, t) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{r} \cdot \nabla)^n \mathbf{E}_{\text{ext}}(\mathbf{0}, t). \quad (5.133)$$

By insertion of the expansion into the expression for the rate of energy transfer to the particle system one obtains

$$\begin{aligned} \frac{dH_{\text{par}}(t)}{dt} &= \int_V \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{E}_{\text{ext}}(\mathbf{r}, t) d^3r \\ &= \left[\int_V \mathbf{J}(\mathbf{r}, t) d^3r \right] \cdot \mathbf{E}_{\text{ext}}(\mathbf{0}, t) \\ &\quad + \left[\int_V \mathbf{J}(\mathbf{r}, t) \mathbf{r} d^3r \right] : \nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t) + \dots, \end{aligned} \quad (5.134)$$

where V is the volume of the mesoscopic particle. The moment expansion scheme for the current density, which was studied in Sect. 5.1, shows that (5.134) can be written as follows:

$$\begin{aligned} \int_V \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{E}_{\text{ext}}(\mathbf{r}, t) d^3r &= \frac{d\mathbf{p}(t)}{dt} \cdot \mathbf{E}_{\text{ext}}(\mathbf{0}, t) \\ &\quad + \left(\frac{d}{dt} \mathbf{Q}(t) + \mathbf{U} \times \mathbf{m}(t) \right) : \nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t) + \dots. \end{aligned} \quad (5.135)$$

If the variation of the external field across the mesoscopic object is negligible the rate of work only depends on the (time derivative) of the electric dipole moment of the object. The second term in (5.135), which takes into account first-order changes in the field, depends on the time derivative of the electric quadrupole moment and on the magnetic dipole moment, and involves various elements of the dyad $\nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t)$.

5.6.2 Rate of Momentum Transfer

The external electromagnetic field ($\mathbf{E}_{\text{ext}}$, $\mathbf{B}_{\text{ext}}$) transfers momentum to the particle system at a rate which can be determined from (2.90) and (2.98) replacing ($\mathbf{E}$, $\mathbf{B}$) in these equations with ($\mathbf{E}_{\text{ext}}$, $\mathbf{B}_{\text{ext}}$). Thus,

$$\frac{d}{dt} \mathbf{P}_{\text{par}}(t) = \int_V (\rho(\mathbf{r}, t) \mathbf{E}_{\text{ext}}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t) \times \mathbf{B}_{\text{ext}}(\mathbf{r}, t)) d^3r. \quad (5.136)$$

By means of the Taylor series expansion for $\mathbf{E}_{\text{ext}}(\mathbf{r}, t)$ (5.133), and a similar one for $\mathbf{B}_{\text{ext}}(\mathbf{r}, t)$, one obtains the following result

$$\begin{aligned} \frac{d}{dt} \mathbf{P}_{\text{par}}(t) = & \left[\int_V \rho(\mathbf{r}, t) d^3r \right] \mathbf{E}_{\text{ext}}(\mathbf{0}, t) + \left[\int_V \mathbf{J}(\mathbf{r}, t) d^3r \right] \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t) \\ & + \left[\int_V \rho(\mathbf{r}, t) \mathbf{r} d^3r \right] \cdot \nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t) \\ & + \left[\int_V \mathbf{J}(\mathbf{r}, t) \mathbf{r} d^3r \right] \cdot \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t) + \cdots, \end{aligned} \quad (5.137)$$

where we in the last term have used the abbreviated notation

$$(\mathbf{A} \cdot \times \mathbf{B} \mathbf{C})_i = \sum_l (A_{jl} B_l C_k - A_{kl} B_l C_j), \quad (5.138)$$

with i, j , and k different, and in cyclic order. The first two terms in (5.137) are proportional to zero-order moments of the charge and current densities, and the following two terms involve the first-order moments of these quantities. The Maxwell equation $\partial \mathbf{B}_{\text{ext}}(\mathbf{r}, t) / \partial t = -\nabla \times \mathbf{E}_{\text{ext}}(\mathbf{r}, t)$ shows that the term proportional to $\mathbf{B}_{\text{ext}}$ depends on first-order spatial derivatives of the electric field just as the third term in (5.137) does. In the moment notation, (5.137) takes the form

$$\begin{aligned} \frac{d}{dt} \mathbf{P}_{\text{par}}(t) = & Q \mathbf{E}_{\text{ext}}(\mathbf{0}, t) + \frac{d\mathbf{p}(t)}{dt} \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t) + \mathbf{p}(t) \cdot \nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t) \\ & + \left(\frac{d}{dt} \mathbf{Q}(t) + \mathbf{U} \times \mathbf{m}(t) \right) \cdot \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t) + \cdots, \end{aligned} \quad (5.139)$$

where $Q = \int_{-\infty}^{\infty} \rho d^3r$ is the total charge of the mesoscopic system. For a globally neutral system $Q = 0$.

5.6.3 Angular Momentum Transfer

In Sect. 2.7.4, the conservation law for the local angular momentum was discussed, and for a system with a fixed number of point particles, (2.140) shows that the rate of which angular momentum is transferred from the electromagnetic field to the particle system is given by

$$\begin{aligned} \frac{d}{dt} \mathbf{I}_{\text{par}}(t) = & \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \frac{d}{dt} (\mathbf{r}_{\alpha}(t) \times \mathbf{p}_{\alpha}(t)) \\ = & \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}(t)) \mathbf{r}_{\alpha}(t) \times \frac{d\mathbf{p}_{\alpha}(t)}{dt}. \end{aligned} \quad (5.140)$$

In a notation which also holds for a continuum description of matter, the rate of angular momentum transfer from an externally impressed field therefore is given by

$$\frac{d}{dt} \mathbf{I}_{\text{par}}(t) = \int_V \mathbf{r} \times [\rho(\mathbf{r}, t) \mathbf{E}_{\text{ext}}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t) \times \mathbf{B}_{\text{ext}}(\mathbf{r}, t)] d^3r, \quad (5.141)$$

as can be realized by means of the Newton–Lorentz equation in (2.30). Taylor expansions of $\mathbf{E}_{\text{ext}}(\mathbf{r}, t)$ and $\mathbf{B}_{\text{ext}}(\mathbf{r}, t)$ around $\mathbf{r} = \mathbf{0}$ now give

$$\begin{aligned} \frac{d}{dt} \mathbf{I}_{\text{par}}(t) = & \left[\int_V \rho(\mathbf{r}, t) \mathbf{r} d^3r \right] \times \mathbf{E}_{\text{ext}}(\mathbf{0}, t) \\ & + \left\{ \int_V [\mathbf{J}(\mathbf{r}, t) \mathbf{r} - (\mathbf{r} \cdot \mathbf{J}(\mathbf{r}, t)) \mathbf{U}] d^3r \right\} \cdot \mathbf{B}_{\text{ext}}(\mathbf{0}, t) \\ & + \left[\int_V \rho(\mathbf{r}, t) \mathbf{r} \mathbf{r} d^3r \right] \cdot \nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t) + \cdots, \end{aligned} \quad (5.142)$$

writing out explicitly only terms which effectively contains up to first-order derivatives in the electric field [remember here that $\partial \mathbf{B}_{\text{ext}}(\mathbf{r}, t) / \partial t = -\nabla \times \mathbf{E}_{\text{ext}}(\mathbf{r}, t)$]. Since $d\mathbf{I}_{\text{par}}(t)/dt$ equals the torque $\mathbf{N}(t) = \mathbf{N}^{(0)}(t) + \mathbf{N}^{(1)}(t) + \cdots$ of the external field on the localized charge distribution, one has to lowest order the well-known result

$$\mathbf{N}^{(0)}(t) = \mathbf{p}(t) \times \mathbf{E}_{\text{ext}}(\mathbf{0}, t). \quad (5.143)$$

The term proportional to $\mathbf{B}_{\text{ext}}(\mathbf{0}, t)$ takes a particularly simple form if the current density is divergence-free. In electrodynamics the current density associated with a pure electron-spin transition satisfies the condition $\nabla \cdot \mathbf{J} = 0$. The spin transition plays a particular role in the theory of spatial photon localization, and we shall study the spin dynamics from a quantum physical point of view in Chap. 20. In magnetostatics, where $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}$, one also has $\nabla \cdot \mathbf{J} = 0$. To see how the term proportional to $\mathbf{B}_{\text{ext}}(\mathbf{0}, t)$ is simplified if $\mathbf{J}(\mathbf{r}, t)$ is divergence-free we make use of the two relations

$$\frac{1}{2} \int_V r^2 \nabla \cdot \mathbf{J}(\mathbf{r}, t) d^3r = - \int_V \mathbf{r} \cdot \mathbf{J}(\mathbf{r}, t) d^3r, \quad (5.144)$$

$$\int_V \mathbf{r} \mathbf{r} \nabla \cdot \mathbf{J}(\mathbf{r}, t) d^3r = - \int_V (\mathbf{J}(\mathbf{r}, t) \mathbf{r} + \mathbf{r} \mathbf{J}(\mathbf{r}, t)) d^3r. \quad (5.145)$$

The correctness of these can be proved by partial integrations over a volume V enclosing the entire current density distribution. Equation (5.144) shows that the term containing $\mathbf{r} \cdot \mathbf{J}$ in (5.142) vanishes for $\nabla \cdot \mathbf{J} = 0$. The integral with $\mathbf{J} \mathbf{r}$ in (5.142) is the sum of magnetic dipole and electric quadrupole tensors; cf. (5.13), (5.15), and (5.16). Equation (5.145) is zero when $\nabla \cdot \mathbf{J} = 0$. Utilizing (5.25) and the

relation $\mathbf{U} \times \mathbf{m}(t) \cdot \mathbf{B}_{\text{ext}}(\mathbf{0}, t) = \mathbf{m}(t) \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t)$ the term proportional to $\mathbf{B}_{\text{ext}}(\mathbf{0}, t)$ thus is reduced to

$$N^{(1)}(t | \nabla \cdot \mathbf{J} = 0) = \mathbf{m}(t) \times \mathbf{B}_{\text{ext}}(\mathbf{0}, t) \quad (5.146)$$

if the current density is divergence-free. The term proportional to $\nabla \mathbf{E}_{\text{ext}}(\mathbf{0}, t)$ is zero when the electric quadrupole moment tensor (given by (5.29)) vanishes.

Chapter 6

Electrodynamic Interaction Between Point Dipoles: Local Fields

In near-field electrodynamics, it is of central importance to study electromagnetic field variations on a length scale (much) shorter than the wavelengths which characterize the given problem. Macroscopic field calculations must therefore be replaced by so-called local-field analyses. Although, in general, quantum physics is required to determine local fields in both macroscopic and mesoscopic media, it is nevertheless of some interest to study such fields on the basis of the classical point-particle model. The importance of the local field cannot be overestimated since a knowledge of this field allows one to predict *all* electrodynamic properties of the medium under study. Local fields can of course only be calculated approximately, even within the framework of the naive classical point-particle picture. In this chapter, we shall see how local fields emerge from multiple scattering among polarizable point-particles occupying fixed positions in space, and we shall begin to understand that the eigenmode concept in electrodynamics in its widest sense is a manifestation of resonance in the local field.

6.1 Multiple ED-Scattering to Infinite Order

Let us now consider the electromagnetic interaction among N electric dipoles located at the fixed positions $\mathbf{r}_i, i = 1, 2, \dots, N$. The system is assumed to be driven by an externally impressed electric field $\mathbf{E}^{\text{ext}}(\mathbf{r}; \omega)$, and the electric field of the i th dipole has the value $\mathbf{E}^{(i)}(\mathbf{r}; \omega)$ at the space point $\mathbf{r}$. The local electric field, $\mathbf{E}(\mathbf{r}; \omega)$, is the sum of the external field and the fields from the various dipoles. Hence,

$$\mathbf{E}(\mathbf{r}; \omega) = \mathbf{E}^{\text{ext}}(\mathbf{r}; \omega) + \sum_{i=1}^N \mathbf{E}^{(i)}(\mathbf{r}; \omega) \quad (6.1)$$

in the space–frequency domain. If the electric dipole moment of particle number i is denoted by $\mathbf{p}_i(\omega)$ one has (see (5.37))

$$\mathbf{E}^{(i)}(\mathbf{r}; \omega) = \mu_0 \omega^2 \mathbf{G}(\mathbf{r} - \mathbf{r}_i; \omega) \cdot \mathbf{p}_i(\omega). \quad (6.2)$$

Together, (6.1) and (6.2) give a relation between the local field at $\mathbf{r}$ and the electric dipole moments of the various particles. If the $\mathbf{p}_i(\omega)$'s were known (prescribed) the local field could easily be determined everywhere in space. At least a part of $\mathbf{p}_i(\omega)$ originates in the local field acting on this dipole. For simplicity it is now assumed that the entire electric dipole moment $\mathbf{p}_i(\omega)$ is induced by the local field $\mathbf{E}(\mathbf{r}; \omega)$ acting on the particle, and that $\mathbf{p}_i(\omega)$ is linearly related to $\mathbf{E}(\mathbf{r}; \omega)$. If the local field is weak and the angular frequency is not close to an inner resonance frequency of the particle, the linearity assumption usually is good. In the following we thus put

$$\mathbf{p}_i(\omega) = \boldsymbol{\alpha}_i(\omega) \cdot \mathbf{E}(\mathbf{r}_i; \omega), \quad i = 1, 2, \dots, N, \quad (6.3)$$

where $\boldsymbol{\alpha}_i(\omega)$ is the electric-dipole polarizability (tensor) of the i th particle. To determine $\boldsymbol{\alpha}_i(\omega)$ most often one needs to carry out some sort of quantum physical calculation (see Chap. 12). Since the inner structure of the particle usually is anisotropic, we expect, as indicated in (6.3), that the $\mathbf{p}_i(\omega) - \mathbf{E}^{\text{ext}}(\mathbf{r}_i; \omega)$ relation is of tensorial character.

By combining (6.1)–(6.3) one obtains the following implicit expression for the local electric field:

$$\mathbf{E}(\mathbf{r}; \omega) = \mathbf{E}^{\text{ext}}(\mathbf{r}; \omega) + \sum_{j=1}^N \mathbf{T}(\mathbf{r} - \mathbf{r}_j; \omega) \cdot \mathbf{E}(\mathbf{r}_j; \omega), \quad (6.4)$$

with

$$\mathbf{T}(\mathbf{r} - \mathbf{r}_j; \omega) = \mu_0 \omega^2 \mathbf{G}(\mathbf{r} - \mathbf{r}_j; \omega) \cdot \boldsymbol{\alpha}_j(\omega). \quad (6.5)$$

It appears from (6.4) that the local field can be determined everywhere in space *provided* this field is known just at the sites of the N dipoles. When saying this I have of course presupposed that the tensor $\mathbf{T}(\mathbf{r} - \mathbf{r}_j; \omega)$ is known. This tensor contains a product of the Green function for the electric field, which is known in explicit form ((3.32) with $\mathbf{R} = \mathbf{r} - \mathbf{r}_j$), and the ED-polarizability of the various particles, which in general is known only approximately. In the quantum physical study of local fields, to be described in Parts II and III of this book, a tensor with a structure similar to that of $\mathbf{T}$ occurs, yet with the so-called transverse propagator taking the place of $\mathbf{G}$ and with $\boldsymbol{\alpha}_j(\omega)$ replaced by the ED-polarizability relating the electric dipole moment to the divergence-free part of the electric field.

In order to obtain the yet unknown electric fields at the locations of the dipoles we set $\mathbf{r} = \mathbf{r}_i$ in (6.4). This gives

$$\mathbf{E}(\mathbf{r}_i; \omega) = \mathbf{E}^{\text{ext}}(\mathbf{r}_i; \omega) + \sum_{j \neq i} \mathbf{T}(\mathbf{r}_i - \mathbf{r}_j; \omega) \cdot \mathbf{E}(\mathbf{r}_j; \omega), \quad (6.6)$$

omitting by *brute force* the term with $j = i$ from the summation. From a physical point of view we thus neglect the radiative reaction the field from the i th dipole has on the motion of the dipole itself. The radiative reaction cannot in general

be neglected, and we will study the effect further within the framework of the microscopic classical theory in Chap. 7. In the quantum theory of near-field electrodynamics, the radiative reaction plays a central role conceptually, and its inclusion in local-field calculations is often necessary from a quantitative point of view as we shall realize later on. In the present context the $j = i$ term must be omitted from the calculations for the following technical reasons: The Green function $\mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega)$ is singular for $\mathbf{r}_i = \mathbf{r}_j$, and the singular behavior is transferred unmodified to $\mathbf{T}(\mathbf{r}_i - \mathbf{r}_j; \omega)$ via (6.5). In turn this fact necessitates that radiative reaction effects must be omitted in advance. Physically, the problem does not originate in the singularity of the Green function, but in the circumstance that we have started with the assumption that particles are point-like entities. Starting from a finite-size particle model the singularity in $\mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega)$ will not be transferred to the relevant new $\mathbf{T}(\mathbf{r}_i - \mathbf{r}_j; \omega)$, which thus will be finite for all $\mathbf{r}_i - \mathbf{r}_j$. A nonsingular $\mathbf{T}$ allows one to incorporate radiative reaction phenomena in the local field calculations.

Let us now return to (6.6), which with the abbreviations $\mathbf{E}(\mathbf{r}_\alpha; \omega) \equiv \mathbf{E}_\alpha$, $\mathbf{E}^{\text{ext}}(\mathbf{r}_\alpha; \omega) \equiv \mathbf{E}_\alpha^{\text{ext}}$, and $\mathbf{T}(\mathbf{r}_\alpha - \mathbf{r}_\beta; \omega) \equiv \mathbf{T}_{\alpha\beta}$, [$\alpha = i, j$], reads

$$\mathbf{E}_i = \mathbf{E}_i^{\text{ext}} + \sum_{j \neq i} \mathbf{T}_{ij} \cdot \mathbf{E}_j. \quad (6.7)$$

Equation (6.7) is an inhomogeneous linear vectorial equation among the N unknown local fields of the sites of the dipoles. By letting the index i run through the values $i = 1, 2, \dots, N$, one generates a set of N inhomogeneous equations among the N unknown local fields at the dipole locations. Once this algebraic set of linear equations has been solved the local field can be determined everywhere in space via (6.4). Using supermatrix notation with

$$\mathcal{E} \equiv \begin{pmatrix} \mathbf{E}_1 \\ \mathbf{E}_2 \\ \vdots \\ \mathbf{E}_n \end{pmatrix}, \quad \mathcal{E}^{\text{ext}} \equiv \begin{pmatrix} \mathbf{E}_1^{\text{ext}} \\ \mathbf{E}_2^{\text{ext}} \\ \vdots \\ \mathbf{E}_n^{\text{ext}} \end{pmatrix}, \quad (6.8)$$

and

$$\mathcal{T} \equiv \begin{pmatrix} \mathbf{0} & \mathbf{T}_{12} & \cdots & \mathbf{T}_{1n} \\ \mathbf{T}_{21} & \mathbf{0} & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathbf{T}_{n1} & \cdots & \cdots & \mathbf{0} \end{pmatrix}, \quad (6.9)$$

the set of algebraic equations can be written in the compact form

$$\mathcal{E} = \mathcal{E}^{\text{ext}} + \mathcal{T} \cdot \mathcal{E}. \quad (6.10)$$

Formally, the solution for $\mathcal{E}$ is given by

$$\mathcal{E} = (\mathcal{U} - \mathcal{T})^{-1} \cdot \mathcal{E}^{\text{ext}}, \quad (6.11)$$

where

$$\mathcal{U} = \begin{pmatrix} U & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & U & & \vdots \\ \vdots & & \ddots & \vdots \\ \mathbf{0} & \cdots & \cdots & U \end{pmatrix} \quad (6.12)$$

is the unit supermatrix of dimension $N \times N$ in vector notation (or $3N \times 3N$ in component notation), and $(\mathcal{U} - \mathcal{T})^{-1}$ is the inverse supermatrix to $(\mathcal{U} - \mathcal{T})$. Within the framework of the point-particle model the expression for $\mathcal{E}$ in (6.11) represents the exact solution for the local field at the electric dipole sites. In the language of multiple scattering, (6.11) corresponds to multiple ED-scattering to infinite order, as we shall realize in the next section.

6.2 ED-Scattering in a Born Series Approach

The exact solution given for the supervector $\mathcal{E}$ in (6.11) can be related to the physics describing all kinds of multiple ED-field scattering between the point-particles. To understand this, let us start from (6.10), and assume that the electromagnetic interaction between the particles is weak. This may for instance be the case if the particles are far from each other, or if the external field only gives rise to small induced dipole moments. In lowest (*zeroth*) order (superscript (0)), the mutual particle interaction is neglected and the local fields thus equals the external fields acting on the various dipoles, i.e.,

$$\mathcal{E}^{(0)} = \mathcal{E}^{\text{ext}}. \quad (6.13)$$

In the next approximation, the interaction between the particles is taken in account, but it is assumed the dipole moments are induced only by the (dominating) external field. In first order (superscript (1)) one therefore gets a supervector

$$\mathcal{E}^{(1)} = \mathcal{E}^{(0)} + \mathcal{T} \cdot \mathcal{E}^{(0)}. \quad (6.14)$$

The approximation $\mathcal{E} = \mathcal{E}^{(1)}$ given by (6.14) is called the first-order Born approximation, and named after Max Born one of the pioneers in the development of quantum physics. In next order (superscript (2)), the $\mathcal{E}$ on the right side of (6.10) is replaced by $\mathcal{E}^{(1)}$, so as to give the second-order Born approximation

$$\mathcal{E}^{(2)} = \mathcal{E}^{(0)} + \mathcal{T} \cdot \mathcal{E}^{(1)}. \quad (6.15)$$

The iterative method outlined above thus relates the n th order solution to the $(n-1)$ th order supervector field as follows:

$$\mathcal{E}^{(n)} = \mathcal{E}^{(0)} + \mathcal{T} \cdot \mathcal{E}^{(n-1)}. \quad (6.16)$$

Working backwards from (6.16) it is readily realized that the n th order approximation to the local fields on the dipole sites is given by

$$\mathcal{E}^{(n)} = \left[\mathcal{U} + \mathcal{T} \cdot \mathcal{T} + \cdots + \underbrace{(\mathcal{T} \cdot \mathcal{T} \cdots \mathcal{T})}_{n \text{ times}} \right] \cdot \mathcal{E}^{\text{ext}}, \quad (6.17)$$

an expression involving only $\mathcal{T}$ and the (prescribed) external supervector field. The iterative procedure in (6.17) is called the Born series approach for finding the solution for the local electric field. The Born series method is well known also in quantum mechanical scattering theory among massive particles. The iterative method of solution is most valuable if the power series in $\mathcal{T}$ converges rapidly. Since, formally

$$(\mathcal{U} - \mathcal{T})^{-1} = \mathcal{U} + \mathcal{T} + \mathcal{T} \cdot \mathcal{T} + \cdots, \quad (6.18)$$

within the domain of convergence for the power series, it appears that the selfconsistent result in (6.11) includes multiple scattering effects to infinite order.

In order to elaborate on the physical aspects of multiple scattering it is convenient to return to (6.7). If one writes down an equation analogous to this with the changes $i \rightarrow j$ and $j \rightarrow i$ in the dummy index notation, and inserts this equation for $\mathbf{E}_j$ into the right side of (6.7), we obtain the expansion

$$\mathbf{E}_i = \mathbf{E}_i^{\text{ext}} + \sum_{j \neq i} \mathbf{T}_{ij} \cdot \mathbf{E}_j^{\text{ext}} + \sum_{j \neq i} \sum_{k \neq j} \mathbf{T}_{ij} \cdot \mathbf{T}_{jk} \cdot \mathbf{E}_k^{\text{ext}} + \cdots \quad (6.19)$$

for the electric field on the i th dipole. It appears from (6.5) that

$$\mathbf{T}_{ij} = \mu_0 \omega^2 \mathbf{G}_{ij} \cdot \boldsymbol{\alpha}_j, \quad (6.20)$$

where $\mathbf{G}_{ij} \equiv \mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega)$, and (6.19) therefore can be written

$$\begin{aligned} \mathbf{E}_i = & \mathbf{E}_i^{\text{ext}} + \mu_0 \omega^2 \sum_{j \neq i} \mathbf{G}_{ij} \cdot \boldsymbol{\alpha}_j \cdot \mathbf{E}_j^{\text{ext}} \\ & + (\mu_0 \omega^2)^2 \sum_{j \neq i} \sum_{k \neq j} \mathbf{G}_{ij} \cdot \boldsymbol{\alpha}_j \cdot \mathbf{G}_{jk} \cdot \boldsymbol{\alpha}_k \cdot \mathbf{E}_k^{\text{ext}} + \cdots. \end{aligned} \quad (6.21)$$

The terms in (6.16) containing the factor $\mu_0 \omega^2$ represent what is called single-scattering events. Thus, the external field acting on particle number j induces in this particle an electric dipole moment $\mathbf{p}_j = \boldsymbol{\alpha}_j \cdot \mathbf{E}_j^{\text{ext}}$. The electric field radiated (scattered) from this dipole attains the value $\mu_0 \omega^2 \mathbf{G}_{ij} \cdot \mathbf{p}_j$ on the location of the i th particle. In the first-order Born approximation, the field on the i th particle hence is the sum of the external field and the single-scattering contributions from the other particles. The terms in (6.21) which have a prefactor $(\mu_0 \omega^2)^2$ are associated with so-called double-scattering processes. The external field on particle number

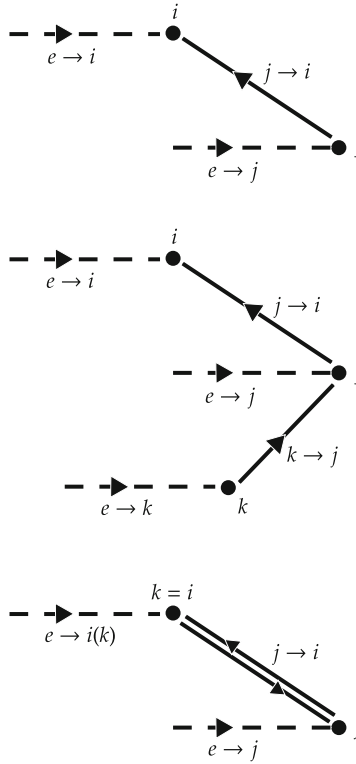


Fig. 6.1 Schematic illustration of single- and double-scattering processes between electric point-dipoles. *Top figure* (single-scattering): An external field e excites dipole j . The field scattered from j , and the external field, excite dipole i . *Middle figure* (double-scattering): The external field (e) excites dipole k . The field scattered from k excites (together with e) dipole j . The field scattered from j (plus the e -field) in turn excites dipole i . *Bottom figure* (special double-scattering): The external field (e) excites dipole i . The scattered field goes to dipole j , and is from j scattered back to i

k induces in this particle an electric dipole moment $\mathbf{p}_k = \alpha_k \cdot \mathbf{E}_k^{\text{ext}}$. The scattered field from this particle reach particle number j with a strength $\mu_0 \omega^2 \mathbf{G}_{jk} \cdot \mathbf{p}_k$, and induces, therefore, an electric dipole moment $\mathbf{p}_j = \mu_0 \omega^2 \alpha_j \cdot \mathbf{G}_{jk} \cdot \mathbf{p}_k$ in this particle. The scattered field reaching the j th particle from the k th particle in turn is scattered once more and this second scattering gives rise to an electric field $\mu_0 \omega^2 \mathbf{G}_{ij} \cdot \mathbf{p}_j$ on dipole number i . Altogether, the sum of the terms in (6.21) which contains the factor $(\mu_0 \omega^2)^2$ represents all double-scattering contributions to the field on particle number i . A special kind of double scattering occurs for $k = i$. In this case, two particles are involved. The first scattering is from i to j , and the second scattering from j back to i . In Fig. 6.1, is shown a graphical illustration of the single- and double-scattering processes.

6.3 Local-Field Resonances

Possible selfsustaining local fields exist if nonvanishing solutions can be obtained for $\mathcal{E}$ in (6.10) in the limit $\mathcal{E}^{\text{ext}} \rightarrow \mathbf{0}$. These selfsustaining solutions I have called local-field resonances for obvious reasons. The resonance condition is in supermatrix notation given by

$$\text{Det}\{\mathcal{U} - \mathcal{T}\} = 0, \quad (6.22)$$

where $\text{Det}\{\dots\}$ means the determinant of $\{\dots\}$. Only in particularly simple cases will it be possible to find explicit solutions to (6.22). Although we have here addressed the local-field resonance issue starting from the microscopic classical theory of electrodynamics these resonances also occur in the macroscopic theory in an average sense, and in quantum physics. All electromagnetic eigenmodes in macroscopic electrodynamics (polaritons, plasmons, radiative and non-radiative wave guide modes, etc.) can be obtained from a field resonance condition. In the quantum mechanics of atoms, molecules and mesoscopic particles the local-field resonance condition for instance gives all the Bohr transition frequencies corrected for local-field effects (Lamb shifts). In a sense, genuine local-field resonances, as given by (6.22), do not exist. Existence requires excitation by some external field $\mathcal{E}^{\text{ext}}$, and the resulting $\mathcal{E}$ is a solution to the inhomogeneous equation in (6.10), and not to the homogeneous equation $\mathcal{E} = \mathcal{T} \cdot \mathcal{E}$, unless $\mathcal{E} \rightarrow \infty$. Infinitely strong $\mathcal{E}$'s do not exist in any medium. Irreversible electronic damping mechanisms and spontaneous emission will always limit the magnitude of the local field more or less. Roughly speaking, local-field resonances are related to minimum values of components of the supermatrix $(\mathcal{U} - \mathcal{T})^{-1}$; cf. (6.11).

Two important kinds of local-field resonances are worth mentioning, and these are related to the general structure of $\mathcal{T}$. From (6.5) and (6.9) it appears that

$$\mathcal{T} = \mathcal{T}(\{\hat{r}_{ij}\}; \{\alpha_i(\omega)\}; \omega), \quad (6.23)$$

where $\{\mathbf{r}_{ij}\}$ and $\{\alpha_i\}$ are the sets of all the interparticle distances and ED-polarizabilities. For a given frequency one can imagine a rearrangement of (some of) the various interparticle distances until the resonance condition in (6.22) is (approximately) fulfilled. These resonances which are called *configurational resonances* are of importance in near-field electrodynamics where microscopic and mesoscopic particles often are moved around. The microscopic classical point-particle model is popular in studies of the electrodynamic interaction between a mesoscopic probe (tip) and a mesoscopic medium or a macroscopic medium in which subwavelength features are of interest. Movements of the probe may lead to configurational resonance. It is obvious that $\mathcal{T}$, and in consequence also the local-field resonances, cannot depend on the position of the center of mass, nor on the overall spatial orientation of the particle system under investigation.

6.4 Two-Particle Interaction

To illustrate the principles used in Sects. 6.1–6.3 to calculate the local field arising from the electrodynamic interaction between an arbitrary number of fixed point particles, we now consider a system with only two electric dipoles. Since

$$\mathcal{U} - \mathcal{T} = \begin{pmatrix} U & -T_{12} \\ -T_{21} & -U \end{pmatrix} \quad (6.24)$$

in the two-particle case, one obtains

$$(\mathcal{U} - \mathcal{T})^{-1} = \begin{pmatrix} (U - T_{12} \cdot T_{21})^{-1} (U - T_{12} \cdot T_{21})^{-1} \cdot T_{12} \\ (U - T_{21} \cdot T_{12})^{-1} (U - T_{21} \cdot T_{12})^{-1} \cdot T_{21} \end{pmatrix}. \quad (6.25)$$

By insertion of (6.25) into (6.11), the local fields, $\mathcal{E} = (E_1, E_2)$, on the two particles can be determined as functions of the external fields, $\mathcal{E}^{\text{ext}} = (\mathcal{E}_1^{\text{ext}}, \mathcal{E}_2^{\text{ext}})$ acting on the dipoles. In the second-order Born approximation, the local fields are given by

$$\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} U + T_{12} \cdot T_{21} & -T_{12} \\ -T_{21} & U + T_{21} \cdot T_{12} \end{pmatrix} \cdot \begin{pmatrix} E_1^{\text{ext}} \\ E_2^{\text{ext}} \end{pmatrix}, \quad (6.26)$$

cf. (6.17). The resonance condition for the local field, given in supermatrix notation in (6.22), takes the form

$$\text{Det}\{\mathcal{U} - \mathcal{T}_{12} \cdot \mathcal{T}_{21}\} = \text{Det}\{\mathcal{U} - \mathcal{T}_{21} \cdot \mathcal{T}_{12}\} = 0. \quad (6.27)$$

The reader may readily prove the equality of the two determinants in (6.27) starting from the two homogeneous vectorial equations $E_1 = T_{12} \cdot E_2$ and $E_2 = T_{21} \cdot E_1$. This equality also ensures that the terms $(U - T_{12} \cdot T_{21})^{-1}$ and $(U - T_{21} \cdot T_{12})^{-1}$ in (6.25) have the same denominators in their respective minor expansions.

Let us now assume that the two particles are identical with a common isotropic ED-polarizability $\alpha(\omega) = \alpha(\omega)U$. From (3.32) it appears that $G(R) = G_{21} \equiv G$, and (6.5) then shows that $T_{12} = T_{21} \equiv T$, where

$$T = \mu_0 \omega^2 \alpha(\omega) G. \quad (6.28)$$

The local-field resonance condition in turn is given by

$$\text{Det}\{U - (\mu_0 \omega^2 \alpha(\omega))^2 G \cdot G\} = 0. \quad (6.29)$$

From the expression in (3.32) for the Green function for the electric field one obtains

$$G(R; \omega) \cdot G(R; \omega) = (g^2 + 2ga)(U - \hat{R} \hat{R}) + a^2(U + 3\hat{R} \hat{R}), \quad (6.30)$$

where $g(R; \omega)$ is the scalar Green function (3.13), and

$$a(R; \omega) = \frac{g(R; \omega)}{iq_0 R} \left(\frac{1}{iq_0 R} - 1 \right). \quad (6.31)$$

In a Cartesian coordinate system with the z -axis along the line joining the two dipoles, the resonance condition takes the form

$$\begin{vmatrix} (\mu_0 \omega^2 \alpha(\omega))^{-2} - (g+a)^2 & 0 & 0 \\ 0 & (\mu_0 \omega^2 \alpha(\omega))^{-2} - (g+a)^2 & 0 \\ 0 & 0 & (\mu_0 \omega^2 \alpha(\omega))^{-2} - 4a^2 \end{vmatrix} = 0. \quad (6.32)$$

For the double-degenerate resonance given by

$$[\mu_0 \omega^2 \alpha(\omega)(g(R; \omega) + a(R; \omega))]^2 = 1, \quad (6.33)$$

the associated electric field lies in a plane perpendicular to the $\hat{\mathbf{R}}$ -direction. For a given distance R between the particles the resonance frequency will in general be complex, i.e., $\omega_{\text{Res}}^{\text{R}} + i\omega_{\text{Res}}^{\text{I}}$, and to compensate for (1) irreversible damping mechanisms associated to the electric dipole polarizability, and (2) radiation losses, the imaginary part ($\omega_{\text{Res}}^{\text{I}}$) of the resonance frequency must be positive. The presence of both $g(R; \omega)$ and $a(R; \omega)$ in (6.33) shows that a double-degenerate local-field resonance may exist independent of whether the dipoles are placed in the near-, mid-, or far-field zone of each other. The electric field associated with the resonance condition

$$[2a(R; \omega)\mu_0 \omega^2 \alpha(\omega)]^2 = 1 \quad (6.34)$$

is directed along the line joining the two electric dipoles, and only if the particles are located in the near- or mid-field zone of each other may such a resonance exist. For $q_0 R \rightarrow 0$, $g(R; \omega) + a(R; \omega) \rightarrow a(R; \omega) \rightarrow -(4\pi q_0^2 R^3)^{-1}$, and for electric dipoles in near-field contact the local-field resonance conditions in (6.33) and (6.34) are reduced to

$$\left(\frac{\eta \alpha(\omega)}{4\pi \epsilon_0 R^3} \right)^2 = 1, \quad (6.35)$$

with $\eta = 1$ for the double-degenerate solution, and $\eta = 2$ for the other one. If the ED-polarizability is real (irreversible damping mechanisms negligible), (6.35) determines the configurational near-field resonance distance R_{Res} as a function of the real angular frequency ω . Self-consistency requires that the condition $q_0 R_{\text{Res}} \ll 1$ must be satisfied.

6.5 Multiple MD- and EQ-Scattering

The electromagnetic interaction between magnetic point dipoles can be treated along the same lines as used to investigate the local field problem for ED-scattering. For a system of N magnetic dipoles placed at the fixed positions $\mathbf{r}_i$, $i = 1, 2, \dots, N$, and driven by an external magnetic field, $\mathbf{B}(\mathbf{r}; \omega)$, satisfies the equation

$$\mathbf{B}(\mathbf{r}; \omega) = \mathbf{B}^{\text{ext}}(\mathbf{r}; \omega) + \sum_{i=1}^N \mathbf{B}^{(i)}(\mathbf{r}; \omega), \quad (6.36)$$

where $\mathbf{B}^{(i)}(\mathbf{r}; \omega)$ is the magnetic field from the i th dipole. If we denote the magnetic dipole moment of particle number i by $\mathbf{m}_i(\omega)$, it appears from (5.46) that

$$\mathbf{B}^{(i)}(\mathbf{r}; \omega) = c_0^{-2} \mu_0 \omega^2 \mathbf{G}(\mathbf{r} - \mathbf{r}_i; \omega) \cdot \mathbf{m}_i(\omega). \quad (6.37)$$

To determine the local magnetic field we need to relate $\mathbf{m}_i(\omega)$ to the magnetic field acting on the dipole. This relation cannot be found from the microscopic Maxwell equations. In most cases, a quantum physical calculation is needed. If the local field is sufficiently weak, and the dipole is not excited in or near resonance, quantum theory leads to a linear constitutive relation

$$\mathbf{m}_i(\omega) = \boldsymbol{\beta}_i(\omega) \cdot \mathbf{B}(\mathbf{r}_i; \omega), \quad (6.38)$$

where $\boldsymbol{\beta}_i(\omega)$ is the magnetic dipole polarizability tensor of the i th dipole. By a combination of (6.36)–(6.38) it is realized that the local magnetic field on the i th dipole is related to the local fields on the other dipoles as follows:

$$\mathbf{B}(\mathbf{r}_i; \omega) = \mathbf{B}^{\text{ext}}(\mathbf{r}_i; \omega) + \sum_{j \neq i} \mathbf{T}_M(\mathbf{r}_i - \mathbf{r}_j; \omega) \cdot \mathbf{B}(\mathbf{r}_j; \omega), \quad (6.39)$$

where

$$\mathbf{T}_M(\mathbf{r}_i - \mathbf{r}_j, \omega) = c_0^{-2} \mu_0 \omega^2 \mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega) \cdot \boldsymbol{\beta}_j(\omega). \quad (6.40)$$

Equation (6.39) is the central equation for determination of the local magnetic field on the dipoles. Its formal analogy to the central equation (6.6) for electromagnetic interaction among electric point dipoles enables one to make the analyses of the multiple MD-scattering, the Born series approach, and the local-field resonances, as described in Sects. 6.1–6.3.

A selfconsistent calculation of the local electric field associated with multiple scattering among electric quadrupoles can be carried out on the basis of (5.55) and the assumed linear relation

$$\mathbf{Q}_i(\omega) = \mathbf{E}(\mathbf{r}_i; \omega) \cdot \boldsymbol{\gamma}_i(\omega) \quad (6.41)$$

between the electric quadrupole moment of the i th dipole and the electric field acting on this dipole. The third rank tensor $\gamma_i(\omega)$ is the so-called electric quadrupole polarizability tensor, a quantity which in general need to be determined by quantum mechanical perturbation theory. The reader may convince herself that the central equation for multiple EQ-scattering has the form

$$\mathbf{E}(\mathbf{r}_i, \omega) = \mathbf{E}^{\text{ext}}(\mathbf{r}_i; \omega) + \sum_{j \neq i} \mathbf{E}(\mathbf{r}_j; \omega) \cdot \mathbf{T}_Q(\mathbf{r}_i - \mathbf{r}_j; \omega), \quad (6.42)$$

where

$$\mathbf{T}_Q(\mathbf{r}_i - \mathbf{r}_j, \omega) = -\mu_0 \omega^2 \gamma_i(\omega) : \nabla \mathbf{G}(\mathbf{r}_i - \mathbf{r}_j; \omega) \quad (6.43)$$

is the second rank tensor coupling the local electric fields at the quadrupole sites i and j .

Chapter 7

Radiation Reaction

In Sect. 2.3, we discussed the solutions to the Maxwell–Lorentz equations, and (2.22) and (2.23) express the microscopic electric and magnetic fields in terms of certain integrals involving the microscopic charge and current densities. If these densities are prescribed (specified) (2.22) and (2.23) represent the physically general solution to the Maxwell–Lorentz equations. In near-field electrodynamics the charge and current densities can seldom be considered as prescribed quantities, but must be related to the local electromagnetic field acting on the particles. Hence, (2.22) and (2.23) only determine the microscopic field in implicit form. In the case of a single point-particle, the Lienard–Wiechert equations ((2.60)–(2.62) and (2.66)–(2.68)) give the electromagnetic field in terms of the velocity and acceleration of the particle. The particle acceleration causes emission of radiation, described by the acceleration fields in (2.62) and (2.68), and a correct treatment of the particle motion must include the reaction of the radiation on this motion. In our treatment of the electromagnetic interaction between point dipoles in Chap. 6, the radiative reaction of the dipole fields was neglected. Incorporation of this effect leads to a change in the local field as we shall see.

7.1 The Nonrelativistic Abraham–Lorentz Equation of Motion

If the emission of radiation is neglected a nonrelativistic point-particle of charge Q and mass m placed in an external and prescribed electromagnetic field ($\mathbf{E}^{\text{ext}}$, $\mathbf{B}^{\text{ext}}$) moves according to the Newton–Lorentz equation

$$m \frac{d\mathbf{v}_Q(t)}{dt} = \mathbf{F}^{\text{ext}}(t), \quad (7.1)$$

where

$$\mathbf{F}^{\text{ext}}(t) = Q [\mathbf{E}^{\text{ext}}(\mathbf{r}_Q(t), t) + \mathbf{v}_Q(t) \times \mathbf{B}^{\text{ext}}(\mathbf{r}_Q(t), t)]. \quad (7.2)$$

Since the particle is accelerated it emits radiation energy at a rate which we below will calculate from the electric and magnetic acceleration fields given in (2.62) and (2.68). To account for this radiative energy loss in the particle's equation of motion, we add a radiative reaction force $\mathbf{F}^{\text{rad}}$ to the Newton–Lorentz equation:

$$m \frac{d\mathbf{v}_Q(t)}{dt} = \mathbf{F}^{\text{ext}}(t) + \mathbf{F}^{\text{rad}}(t). \quad (7.3)$$

In some approximate and time-averaged sense, we determine $\mathbf{F}^{\text{rad}}(t)$ via the radiative power emitted by the particle in the manner discussed below. In the nonrelativistic limit the electric acceleration field in (2.62) reduces to

$$\mathbf{E}_{\text{acc}}(\mathbf{r}, t) = \frac{Q}{4\pi\epsilon_0} \frac{1}{c_0^2 R} \hat{\mathbf{R}} \times (\hat{\mathbf{R}} \times \dot{\mathbf{v}}_Q), \quad (7.4)$$

and the associated magnetic field follows from

$$\mathbf{B}_{\text{acc}}(\mathbf{r}, t) = \frac{1}{c_0} \hat{\mathbf{R}} \times \mathbf{E}_{\text{acc}}(\mathbf{r}, t), \quad (7.5)$$

see (2.68). If the angle between the acceleration vector, $\dot{\mathbf{v}}_Q(t)$, and the direction from the charge to the point of observation, $\hat{\mathbf{R}}(t)$, is denoted θ , the electromagnetic Poynting vector in (2.114) becomes

$$\mathbf{S}(\mathbf{r}, t) = \frac{Q^2}{16\pi^2\epsilon_0 c_0^3} \frac{\dot{\mathbf{v}}_Q^2 \sin^2 \theta}{R^2} \hat{\mathbf{R}}. \quad (7.6)$$

The total instantaneous power radiated, $P(t)$, is obtained by integrating the scalar product $\mathbf{S} \cdot \hat{\mathbf{R}}$ over the entire solid angle. Thus,

$$P(t) = \int_0^{2\pi} \int_0^\pi \mathbf{S}(\mathbf{r}, t) \cdot \hat{\mathbf{R}} R^2 \sin \theta d\theta d\phi, \quad (7.7)$$

and finally

$$P(t) = \frac{Q^2 \dot{\mathbf{v}}_Q^2(t)}{6\pi\epsilon_0 c_0^3}. \quad (7.8)$$

The result in (7.8) is the well known Larmor formula for a nonrelativistic, accelerated charge. The negative of the work carried out on the particle by the radiative reaction force in the time interval $t_1 < t < t_2$ we now demand to be equal to the power radiated in that time. Hence,

$$-\int_{t_1}^{t_2} \mathbf{F}^{\text{rad}}(t) \cdot \mathbf{v}_Q(t) dt = \frac{Q^2}{6\pi\epsilon_0 c_0^3} \int_{t_1}^{t_2} \dot{\mathbf{v}}_Q(t) \cdot \dot{\mathbf{v}}_Q(t) dt. \quad (7.9)$$

By integration of the second integral by parts one yields

$$\int_{t_1}^{t_2} \left[\mathbf{F}^{\text{rad}}(t) - \frac{Q^2}{6\pi\epsilon_0 c_0^3} \ddot{\mathbf{v}}_Q(t) \right] \cdot \mathbf{v}_Q(t) dt = -\frac{Q^2}{6\pi\epsilon_0 c_0^3} [\dot{\mathbf{v}}_Q \cdot \mathbf{v}_Q]_{t_1}^{t_2}. \quad (7.10)$$

If the motion is such that $\dot{\mathbf{v}}_Q \cdot \mathbf{v}_Q = 0$ at $t = t_1$ and $t = t_2$ (or this product just has the same value at the two times), we have

$$\int_{t_1}^{t_2} \left[\mathbf{F}^{\text{rad}}(t) - \frac{Q^2}{6\pi\epsilon_0 c_0^3} \ddot{\mathbf{v}}_Q(t) \right] \cdot \mathbf{v}_Q(t) dt = 0. \quad (7.11)$$

For a harmonic oscillator $\mathbf{v}_Q$ and $\dot{\mathbf{v}}_Q$ will be almost periodic functions when $\mathbf{F}^{\text{rad}}(t)$ is very small. Integration over an integral number of periods then leads to (7.11). If (7.11) is (approximately) correct, it is permissible to identify the radiative reaction force as

$$\mathbf{F}^{\text{rad}}(t) = \frac{Q^2}{6\pi\epsilon_0 c_0^3} \ddot{\mathbf{v}}_Q(t). \quad (7.12)$$

By inserting (7.12) into (7.3) we obtain the modified Newton–Lorentz equation

$$m(\dot{\mathbf{v}}_Q(t) - \tau_0 \ddot{\mathbf{v}}_Q(t)) = \mathbf{F}^{\text{ext}}(t), \quad (7.13)$$

where

$$\tau_0 = \frac{Q^2}{6\pi\epsilon_0 m c_0^3} = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3m c_0^3} \quad (7.14)$$

is the so-called characteristic time. Roughly speaking, radiation reaction effects are only crucial in the nonrelativistic domain if the relative change in the particle acceleration is appreciable on a time scale comparable to (or shorter than) τ_0 . Equation (7.13) is often called the Abraham–Lorentz equation of motion. The longest characteristic time for charged particles is for electrons, where $\tau_0 \approx 6.3 \cdot 10^{-24}$ s. In such a short time, light travels a distance of $\approx 1.9 \cdot 10^{-15}$ m in free space.

The Abraham–Lorentz equation for the particle velocity is of second order in time, rather than first, as dynamical equations of motions usually are. In the absence of the external force (7.13) admits not only the free-particle solution $\dot{\mathbf{v}}_Q(t) = \mathbf{0}$, but also an unphysical “runaway” solution $\dot{\mathbf{v}}_Q(t) = \dot{\mathbf{v}}_Q(0) \exp(t/\tau_0)$. Since the external field always will be nonvanishing only in a finite time interval, the particle is asymptotically free and moves in uniform motion (law of inertia). This is expressed in terms of the following asymptotic condition on the acceleration [130]:

$$\lim_{|t| \rightarrow \infty} \mathbf{a}(t) = \mathbf{0}. \quad (7.15)$$

It should be emphasized that the condition in (7.15) is an essential (indispensable) part of the description, and not “just” an “arbitrarily” imposed condition valid, e.g., for a typical scattering event. To obtain the explicit solution for the particle acceleration $\mathbf{a}_Q(t) = \dot{\mathbf{v}}_Q(t)$ from (7.13), and the condition in (7.15), (7.13) is multiplied by the integrating factor $\exp(-t/\tau_0)$. This gives upon a slight rearrangement

$$\frac{d}{dt} \left(e^{-t/\tau_0} \mathbf{a}_Q(t) \right) = -(m\tau_0)^{-1} e^{-t/\tau_0} \mathbf{F}^{\text{ext}}(t). \quad (7.16)$$

The asymptotic condition in (7.15) implies the weaker condition

$$\lim_{t \rightarrow \infty} \left(e^{-t/\tau_0} \mathbf{a}_Q(t) \right) = \mathbf{0}, \quad (7.17)$$

and integration of (7.16) between t and ∞ therefore gives a particle acceleration

$$\mathbf{a}_Q(t) = (m\tau_0)^{-1} e^{t/\tau_0} \int_t^\infty e^{-t'/\tau_0} \mathbf{F}^{\text{ext}}(t') dt'. \quad (7.18)$$

By change of integration variable from t' to $\alpha = (t' - t)/\tau_0$, (7.18) takes the form

$$m\mathbf{a}_Q(t) = \int_0^\infty e^{-\alpha} \mathbf{F}^{\text{ext}}(t + \alpha\tau_0) d\alpha. \quad (7.19)$$

Equation (7.19) relates the particle acceleration to the external force in a timely nonlocal manner. Thus, $\mathbf{a}_Q(t)$ depends on the force not only at time t but also at all later times. Does this nonlocal time behavior constitute a violation of causality? If causality means predictability, (7.19) certainly is causal since the external forces are given for all future time and not affected by the particle motion. The (nonrelativistic) equation of motion is also causal in the sense that the particle velocity never exceeds the vacuum speed of light. A causality violation in the sense of so-called preacceleration is in principle implied. Thus, if the external force is assumed to be switched on at time $t = t_0$, (7.19) shows that a nonvanishing particle acceleration at times $t < t_0$ is possible. Equation (7.19) therefore seems to violate causality in the sense that advanced effects do occur. Advanced effects correspond to signals sent backward in time. The presence of the preacceleration effect must be taken with a grain of salt. The preacceleration effect occurs at times of the order $\tau_0 \approx 10^{-23}$ s, or less, and to observe such an effect the external force must be switched on over a time interval $\lesssim \tau_0$. No classical interactions can be turned on in such a short time, and the whole question of preacceleration lies outside the domain of classical physics. In view of the fact that the radiative reaction force was determined in some approximate and time-averaged sense it is perhaps not surprising that the Abraham–Lorentz equation of motion predicts the doubtful preacceleration phenomenon. The expression given in (7.12) for the radiative reaction force is however quite useful in physical optics, e.g., because it gives rise to an important contribution to the electric dipole polarizability; see Sect. 7.2.

The smallness of τ_0 suggest that good approximate solutions to (7.19) may be obtained expanding the external force in a power series around $t = t$, i.e.,

$$\mathbf{F}^{\text{ext}}(t + \alpha\tau_0) = \sum_{n=0}^{\infty} \frac{(\alpha\tau_0)^n}{n!} \frac{d^n \mathbf{F}^{\text{ext}}(t)}{dt^n}. \quad (7.20)$$

By insertion of (7.20) into (7.19), and use of the formula

$$\int_0^{\infty} \alpha^n e^{-\alpha} d\alpha = n!, \quad (7.21)$$

the Abraham–Lorentz equation of motion takes the form

$$m\mathbf{a}_Q(t) = \sum_{n=0}^{\infty} \tau_0^n \frac{d^n \mathbf{F}^{\text{ext}}(t)}{dt^n}. \quad (7.22)$$

To lowest order ($n = 0$) (7.22) reduces to the Newton–Lorentz equation in (7.1), and in the next order one obtains

$$m\mathbf{a}_Q(t) = \mathbf{F}^{\text{ext}}(\mathbf{r}_Q(t), t) + \tau_0 \frac{\partial \mathbf{F}^{\text{ext}}(\mathbf{r}_Q(t), t)}{\partial t} + \tau_0 (\mathbf{v}_Q(t) \cdot \nabla) \mathbf{F}^{\text{ext}}(\mathbf{r}_Q(t), t), \quad (7.23)$$

since $d\mathbf{F}^{\text{ext}}/dt = \partial \mathbf{F}^{\text{ext}}/\partial t + (\mathbf{v}_Q \cdot \nabla) \mathbf{F}^{\text{ext}}$. In the nonrelativistic regime, (7.23) can be used to account for small radiative reaction effects. The importance of the radiative correction to the Newton–Lorentz equation only for external forces varying appreciably on the τ_0 time scale can be seen directly transferring (7.13) (or (7.19)) to the frequency domain. A Fourier integral transformation readily gives

$$m\mathbf{a}_Q(\omega) = \frac{\mathbf{F}^{\text{ext}}(\omega)}{1 + i\omega\tau_0}, \quad (7.24)$$

remembering that the transform of $\dot{\mathbf{a}}_Q(t)$ is $-i\omega\mathbf{a}_Q(\omega)$. It appears from (7.24) that only if the external field contains frequency components $\omega \gtrsim \tau_0^{-1}$ will the radiative correction modify the particle motion strongly. In the electron case, a light signal in the characteristic time τ_0 will travel a distance $c_0\tau_0 = 2R^{\text{cl}}/3$, where

$$R^{\text{cl}} = \frac{e^2}{4\pi\epsilon_0 mc_0^2} \quad (7.25)$$

is the classical (Thomson) radius of the electron (charge $-e$) [165, 166]. From the point of view of the Abraham–Lorentz model an appreciable relative change in the particle acceleration requires that the external force varies across the spatial domain of the Thomson electron.

7.2 Damping Force on Electric and Magnetic Dipoles

7.2.1 Bare and Dressed Electric-Dipole Polarizability

Let us consider the motion of a charged point-particle elastically bound to an infinitely heavy point particle, and subjected to a prescribed electric field $\mathbf{E}_0$. For simplicity we assume that the binding force is isotropic with a spring constant $m\omega_0^2$, ω_0 being the resonance frequency of the freely (no coupling to the radiation field) oscillating particle. In the present case, the external field in the Abraham–Lorentz equation of motion

$$m\ddot{\mathbf{r}}_Q(t) = \mathbf{F}^{\text{ext}}(\mathbf{r}_Q(t), t) + m\tau_0\ddot{\ddot{\mathbf{r}}}_Q(t) \quad (7.26)$$

is given by

$$\mathbf{F}^{\text{ext}}(\mathbf{r}_Q(t), t) = Q\mathbf{E}_0(\mathbf{r}_Q(t), t) - m\omega_0^2\mathbf{r}_Q(t). \quad (7.27)$$

Written in the form given in (7.22) it appears that the Abraham–Lorentz equation of motion in general is nonlinear and contains terms in which the spatial variation (dispersion) in the external force occurs. Even if radiative reaction effects are included in lowest order only (7.23), a nonlinear and spatially dispersive term $\tau_0(\dot{\mathbf{r}}_Q \cdot \nabla)\mathbf{F}^{\text{ext}}$ is present. Being interested here in the damping force in the electric dipole limit, the spatial variation in the impressed field is negligible a priori, i.e., $\mathbf{E}_0(\mathbf{r}_Q(t), t) = \mathbf{E}_0(t)$. In the ED-limit, the Abraham–Lorentz equation thus is reduced to

$$m(\ddot{\mathbf{r}}_Q(t) + \omega_0^2\mathbf{r}_Q(t)) = Q(\mathbf{E}_0(t) + \mathbf{E}_{\text{RR}}(t)), \quad (7.28)$$

where

$$\mathbf{E}_{\text{RR}}(t) = \frac{1}{4\pi\epsilon_0} \frac{2Q}{3c_0^3} \ddot{\ddot{\mathbf{r}}}_Q(t), \quad (7.29)$$

is the electric radiation reaction (RR) field. For an elastically bound particle there is in the ED-limit no need to resort to iterative (approximate) techniques when solving the Abraham–Lorentz equation. Written in the form given in (7.28) one may regard the oscillator as undamped but subject to the total field, $\mathbf{E}_0 + \mathbf{E}_{\text{RR}}$. In the frequency domain, (7.28) takes the algebraic form

$$m(\omega_0^2 - \omega^2 - i\omega^3\tau_0)\mathbf{r}_Q(\omega) = Q\mathbf{E}_0(\omega). \quad (7.30)$$

Since the electric dipole moment of the particle, $Q\mathbf{r}_Q(\omega)$, is related to the impressed field by $Q\mathbf{r}_Q(\omega) = \boldsymbol{\alpha}(\omega) \cdot \mathbf{E}_0(\omega)$, (7.30) readily gives the following result for the here isotropic ED-polarizability:

$$\alpha(\omega) = \frac{Q^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega^3\tau_0}. \quad (7.31)$$

The polarizability in (7.31) is called the *dressed* ED-polarizability because the effect of the radiation reaction field is included in the particle's polarizability, and thus not considered as an “externally” impressed field effect. In our study of multiple scattering among a system of electric dipoles in Sects. 6.1–6.4 it is the dressed ED-polarizability which enters the analysis; see (6.3). If one defines a so-called *bare* ED-polarizability α_0 , via the particle's response to the total field, $\mathbf{E}_0 + \mathbf{E}_{\text{RR}}$, i.e., as follows: $Q\mathbf{r}_Q(\omega) = \boldsymbol{\alpha}(\omega) \cdot (\mathbf{E}_0(\omega) + \mathbf{E}_{\text{RR}}(\omega))$, (7.30) leads to the isotropic bare ED-polarizability

$$\alpha_0(\omega) = \frac{Q^2}{m} \frac{1}{\omega_0^2 - \omega^2}. \quad (7.32)$$

The bare and dressed ED-polarizabilities are related by the equation

$$\alpha^{-1}(\omega) = \alpha_0^{-1}(\omega) - \frac{i}{4\pi\epsilon_0} \frac{2}{3} \left(\frac{\omega}{c_0} \right)^3. \quad (7.33)$$

Since the radiation reaction field inevitably is a part of the particle's “inner” dynamics it is the dressed ED-polarizability which is the observable quantity in (near-field) electrodynamics. Figure 7.1 shows a graphical illustration of the scattering of an external field from a point-particle in the bare and dressed polarization approaches.

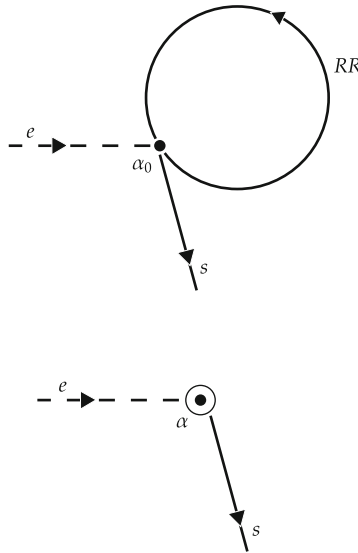


Fig. 7.1 Graphical illustration of the scattering of an external field (denoted by e) from a polarizable point-like particle. *Top figure*: If the particle dynamics is described by (the unobservable) *bare* electric-dipole polarizability α_0 , the scattered field (denoted by s) originates in the particle's response to the sum of the external field and the radiation reaction field (indicated by RR). *Bottom figure*: The radiation reaction field renormalizes the ED-polarizability from its field-undressed value α_0 to the field-dressed value α . The scattered field (s) now is pictured as a response to the external field (e) alone

7.2.2 Near-Zone Electric Green Function: Radiation Damping

In our study of the near-field part of the (electric) Green function in Sect. 3.3.4 it was mentioned that in many cases it is justified to neglect the small phase shift in the $\exp(i q_0 R)$ -factor, and thus replace this factor by unity. By doing so (3.40) reduces to the quasi-static result in (3.41). I shall demonstrate below that only by retaining certain small phase shifts in the electric Green function near $R = 0$ can one account for the radiation damping. Since the effect originates in the back-action of the emitted dipole field on the particle itself it is understandable that it is the phase shifts near (on) the particle which are of interest. We do expect beforehand that phase shifts must be included in some sense since the radiation reaction gives an “out-of-phase” contribution to the bare ED-polarizability. Perhaps, it is not so obvious that small phase shifts in the mid- and far-field parts of the Green function *must* be included in addition to the near-field phase shift to account correctly for the radiation damping.

Let us now return to the expression given in (3.32) for the dyadic Green function belonging to the electric field, and to alleviate the notation let us introduce the following abbreviations: $i q_0 R = \eta$, $[i q_0/(4\pi)](\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}) = \mathbf{F}$, $[i q_0/(4\pi)](\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) = \mathbf{M}$ or $\mathbf{N}$. The notations $\mathbf{F}$, $\mathbf{M}$, and $\mathbf{N}$ refer to far, mid and near field. With these abbreviations the Green function in (3.32) is

$$\mathbf{G} = \frac{e^\eta}{\eta^3} (\eta^2 \mathbf{F} - \eta \mathbf{M} + \mathbf{N}). \quad (7.34)$$

A power series expansion of $\exp(\eta)$ around $\eta = 0$ gives, keeping terms to third order in η in the nominator of (7.34), the following result for the Green function near $R = 0$:

$$\begin{aligned} \mathbf{G} = \frac{1}{\eta^3} & \left[(\eta^2 + \eta^3) \mathbf{F} - (\eta - \eta^2 - \frac{1}{2} \eta^3) \mathbf{M} \right. \\ & \left. + (1 + \eta + \frac{1}{2} \eta^2 + \frac{1}{6} \eta^3) \mathbf{N} + \mathcal{O}(\eta^4) \right]. \end{aligned} \quad (7.35)$$

Terms in-phase with the quasi-static Green function are of even order in η in the nominator of (7.35), and terms out-of-phase are of uneven order. Near $R = 0$ the dominating “in-phase” term to $\mathbf{G}$ is $\mathbf{N}/\eta^3$ as we already know. The terms proportional to η in the denominator of (7.35) cancel, and the dominating “out-of-phase” term to $\mathbf{G}$ hence comes from the η^3 -terms in the nominator. The near-, mid-, and far-field parts of $\mathbf{G}$ all contribute to this term, and it is given by

$$\mathbf{F} - \frac{1}{2} \mathbf{M} + \frac{1}{6} \mathbf{N} = \frac{i q_0}{6\pi} \mathbf{U}. \quad (7.36)$$

Near $R = 0$, the electric Green function may thus be approximated by

$$\mathbf{G}(\mathbf{R}; \omega) \cong \frac{3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U}}{4\pi q_0^2 R^3} + \frac{iq_0}{6\pi} \mathbf{U}. \quad (7.37)$$

Note that the “out-of phase” term in (7.37) is independent of R , and will thus be constant in space across the domain of the microscopic or mesoscopic particles under study. The associated electric field is precisely the radiation reaction field of an electric dipole, i.e.,

$$\mathbf{E}_{\text{RR}}(\omega) = \frac{i}{4\pi\epsilon_0} \frac{2}{3} \left(\frac{\omega}{c_0} \right)^3 \mathbf{p}(\omega), \quad (7.38)$$

as a comparison to (7.29) readily shows, remembering that $\mathbf{p}(\omega) = Q\mathbf{r}_Q(\omega)$.

7.2.3 Magnetic Radiation Damping

The Green function for the magnetic field (3.33) has no near-field part, and near $R = 0$ the dominating term is the mid-field contribution given in (3.39), with $\exp(iq_0 R) = 1$. To obtain the dominating “out-of-phase” term, and to see how the far- and mid-field terms of the magnetic Green function contribute to this term, let us again alleviate the notation by the following abbreviations: $iq_0 R = \eta$, $[iq_0/(4\pi)]\mathbf{U} \times \hat{\mathbf{R}} = \mathbf{F}_M$ or $\mathbf{M}_M$. In the magnetic Green function,

$$\mathbf{G}_M = \frac{e^\eta}{\eta^2} (\eta \mathbf{F}_M - \mathbf{M}_M), \quad (7.39)$$

we now make the power expansion of $\exp(\eta)$ around $\eta = 0$, as before. This gives

$$\mathbf{G}_M = \frac{1}{\eta^2} \left[(\eta + \eta^2 + \frac{1}{2}\eta^3) \mathbf{F}_M - (1 + \eta + \frac{1}{2}\eta^2 + \frac{1}{6}\eta^3) \mathbf{M}_M + \mathcal{O}(\eta^4) \right]. \quad (7.40)$$

The nominator of the dominating “out-of-phase” term thus is

$$\eta^3 \left(\frac{1}{2} \mathbf{F}_M - \frac{1}{6} \mathbf{M}_M \right) = \frac{1}{3} \eta^3 \mathbf{F}_M, \quad (7.41)$$

and near $R = 0$ the Green function for the magnetic field hence can be approximated by the expression

$$\mathbf{G}_M(\mathbf{R}; \omega) = \frac{\mathbf{U} \times \hat{\mathbf{R}}}{4\pi R} \left[-\frac{1}{iq_0 R} + \frac{1}{3}(iq_0 R)^2 \right]. \quad (7.42)$$

The “out-of phase” term thus varies proportional to R near $R = 0$, and does not contribute to the radiation damping on an electric dipole.

The duality between the electric and magnetic fields, expressed for dipole fields through (5.37), (5.38), (5.46), and (5.47), implies that the electric field of a magnetic dipole does not contribute to the radiation damping of such a dipole. A comparison of (5.37) and (5.46), in combination with the result in (7.37) and (7.38), immediately show that the magnetic radiation reaction field on a magnetic dipole is given by

$$\mathbf{B}_{\text{RR}}(\omega) = \frac{i\mu_0}{4\pi} \frac{2}{3} \left(\frac{\omega}{c_0} \right)^3 \mathbf{m}(\omega). \quad (7.43)$$

7.3 The Relativistic Lorentz–Dirac Equation of Motion

In the present section, we shall briefly discuss how the relativistic equation of motion of a charged point particle is expected to be modified by the particle’s own field. In the present chapter, we chose the elements of the diagonal metric tensor $g_{\mu\nu}$ [$\mu, \nu = 0, 1, 2, 3$] as follows: $-g_{00} = g_{11} = g_{22} = g_{33} = +1$.

7.3.1 Manifestly Covariant Expression for the Energy–Momentum Radiation Rate

In the instantaneous rest frame of the particle the Larmor formula for the radiated power (7.8) must necessarily be exact since the particle velocity ($\mathbf{v}_Q \equiv \mathbf{v}$, below) is zero in this frame, eo ipsi. It is useful now to express the instantaneous power emission in terms of the four-acceleration in the rest frame. Since the contravariant four-acceleration of the particle in an arbitrary inertial frame is given by

$$\{a^\mu\} = \left\{ \frac{dw^\mu}{d\tau} \right\} = \left(c_0 \frac{d\gamma}{d\tau}, \frac{d}{d\tau}(\gamma\mathbf{v}) \right), \quad (7.44)$$

where $\{w^\mu\} = \gamma(c_0, \mathbf{v})$ is the four-velocity, and τ is the proper time, the four-acceleration in the rest frame (superscript (0)) is

$$\{a^{\mu(0)}\} = \left\{ \frac{dw^{\mu(0)}}{d\tau} \right\} = \left(0, \frac{d\mathbf{v}}{dt^{(0)}} \right), \quad (7.45)$$

remembering that $\gamma = 1$, and $d\tau = dt^0$. With the “summation over repeated indices”-convention in force ($\mu = 0, 1, 2, 3$) the scalar product of the covariant ($\{a_\mu^{(0)}\}$) and contravariant ($\{a^{\mu(0)}\}$) rest frame acceleration becomes

$$a_\mu^{(0)} a^{\mu(0)} = \dot{\mathbf{v}}^2, \quad (7.46)$$

where the dot stands for differentiation with respect to the proper time. In view of (7.46) the Larmor formula for the radiated power [167] can be written in the form

$$P = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0^3} a_\mu^{(0)} a^{\mu(0)}. \quad (7.47)$$

If the instantaneous relativistic energies of the particle in the arbitrary frame and rest frame are denoted by E and E^0 , the relations $E = \gamma E^0 (= \gamma m c_0^2)$ and $dt = \gamma d\tau$ imply that the radiative rate of energy loss

$$P = -\frac{dE^{(0)}}{d\tau} = -\frac{dE}{dt} \quad (7.48)$$

is a Lorentz invariant. To generalize (7.47) to an arbitrary inertial frame we therefore just need to replace the rest frame accelerations by the corresponding accelerations in the arbitrary frame. Since the scalar product of the covariant and contravariant four-accelerations is a Lorentz invariant, the radiated electromagnetic power can be expressed in the manifestly covariant form

$$P = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0^3} a_\mu a^\mu. \quad (7.49)$$

When expressed in terms of the three-vector velocity ($\mathbf{v} = c_0 \boldsymbol{\beta}$) and acceleration ($\dot{\mathbf{v}} = c_0 \dot{\boldsymbol{\beta}}$) the generalized Larmor formula is also called the Liénard formula. To rewrite (7.49) in three-vector notation, one utilizes (7.44) and the relation $d\tau = \gamma^{-1} dt$ to obtain

$$a_\mu a^\mu = \gamma^2 c_0^2 \left\{ \left[\frac{d}{dt} (\gamma \boldsymbol{\beta}) \right]^2 - \left(\frac{d\gamma}{dt} \right)^2 \right\}, \quad (7.50)$$

and thereafter

$$a_\mu a^\mu = \gamma^6 c_0^2 \left[\dot{\boldsymbol{\beta}}^2 - (\boldsymbol{\beta} \times \dot{\boldsymbol{\beta}})^2 \right]. \quad (7.51)$$

The relativistic Lienard formula for the radiated power thus takes the well known form

$$P = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0} \frac{\dot{\boldsymbol{\beta}}^2 - (\boldsymbol{\beta} \times \dot{\boldsymbol{\beta}})^2}{(1 - \beta^2)^3}. \quad (7.52)$$

In the nonrelativistic limit ($\boldsymbol{\beta} \rightarrow \mathbf{0}$), we regain the Larmor expression in (7.8), of course.

The derivative of the particle's contravariant four-momentum $\{p^\mu\} = (E/c_0, \mathbf{p})$ with respect to the proper time, given by

$$\left\{ \frac{dp^\mu}{d\tau} \right\} = m \left\{ \frac{dw^\mu}{d\tau} \right\} = \left(\frac{1}{c_0} \frac{dE}{d\tau}, \frac{d\mathbf{p}}{d\tau} \right), \quad (7.53)$$

or equivalently

$$\left\{ \frac{dp^\mu}{d\tau} \right\} = \frac{1}{\gamma} \left(\frac{1}{c_0} \frac{dE}{dt}, \frac{d\mathbf{p}}{dt} \right), \quad (7.54)$$

is a Lorentz invariant vector. In (7.53), m is the rest mass of the particle. In the instantaneous rest frame of the particle the radiated electromagnetic field carries no net momentum, cf. the symmetry of the Poynting vector in (7.6). The change in the particle's momentum $d\mathbf{p}/dt$ therefore is zero (as is the three-momentum itself) in the rest frame. In view of (7.48), we thus have in the instantaneous rest frame

$$\left\{ \frac{dp^{\mu(0)}}{d\tau} \right\} = \left(-\frac{P}{c_0}, \mathbf{0} \right). \quad (7.55)$$

A Lorentz transformation (boost) to the frame where the particle has the velocity $\mathbf{v} = c_0 \boldsymbol{\beta}$ readily gives

$$\left\{ \frac{dp^\mu}{d\tau} \right\} = -\frac{P}{c_0^2} (\gamma c_0, \gamma c_0 \boldsymbol{\beta}) \quad (7.56)$$

and thus in terms of the four-velocity

$$\left\{ \frac{dp^\mu}{d\tau} \right\} = -\frac{P}{c_0^2} \{w^\mu\}. \quad (7.57)$$

By insertion of the expression given for the radiated power in (7.47) we finally obtain the following manifestly covariant expression for the rate of energy–momentum transfer to the radiated field:

$$-\left\{ \frac{dp^\mu}{d\tau} \right\} = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0^5} \frac{dw_\nu}{d\tau} \frac{dw^\nu}{d\tau} w^\mu, \quad (7.58)$$

again with the summation over repeated indices kept implicit.

7.3.2 Rest-Mass Preserving Interactions

The nonrelativistic Abraham–Lorentz equation of motion (7.13) deviates from the Newton–Lorentz equation by just a radiation reaction term (7.12). If only such a correction (7.58) was present in the relativistic domain, an accelerated charged point-particle (electron, muon,...) would lose rest mass in the radiation process. Since electrons, for instance, do emerge from radiation processes with their rest masses intact, there must be some extra reaction present to cancel the rest-mass changing radiation. In the present context, the question of rest-mass conservation is adequately studied starting from the expression $w_\mu dp^\mu/d\tau = m^{-1} p_\mu dp^\mu/d\tau$. It is readily shown that

$$p^\mu \frac{dp_\mu}{d\tau} = p_\mu \frac{dp^\mu}{d\tau}, \quad (7.59)$$

and from this relation one obtains

$$w_\mu \frac{dp^\mu}{d\tau} = \frac{1}{2m} \frac{d}{d\tau} (p_\mu p^\mu). \quad (7.60)$$

By means of the energy–momentum relation

$$p_\mu p^\mu = -(mc_0)^2, \quad (7.61)$$

equation (7.60) leads to the result

$$w_\mu \frac{dp^\mu}{d\tau} = -c_0^2 \frac{dm}{d\tau}. \quad (7.62)$$

For rest-mass preserving interactions one therefore has $w_\mu dp^\mu/d\tau = 0$. For a general (nonrelativistic) Newtonian force $\mathcal{F}$, always satisfying the equations $d\mathbf{p}/d\tau = \gamma \mathcal{F}$ and (consequently) $dE/d\tau = \gamma \mathbf{v} \cdot \mathcal{F}$, the equation of motion for the energy–momentum four-vector is

$$\left\{ \frac{dp^\mu}{d\tau} \right\} = \gamma (\boldsymbol{\beta} \cdot \mathcal{F}, \mathcal{F}), \quad (7.63)$$

and in this case the rest-mass preserving condition

$$w_\mu \frac{dp^\mu}{d\tau} = 0 \quad (7.64)$$

holds, as the reader readily may show using $\{w_\mu\} = \gamma c_0(-1, \boldsymbol{\beta})$. In electromagnetic interactions via the Lorentz force $\mathcal{F} = Q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$ the rest mass of the point particle is a conserved quantity.

The rate of energy–momentum transfer to the radiation (rad) field, given in (7.57), does not conserve the rest mass because

$$w_\mu \left(\frac{dp^\mu}{d\tau} \right)_{\text{rad}} = P(\neq 0), \quad (7.65)$$

remembering that $w_\mu w^\mu = -c_0^2$. Perhaps, this result is not surprising due to the fact that the particle can only give up energy and momentum in proportions consistent with the dispersion relation $p_\mu p^\mu = -(mc_0)^2$, whereas the radiation field takes up proportions satisfying $p_\mu p^\mu = 0$ (in relativistic wave mechanics this is the dispersion relation for a massless particle, here a photon).

7.3.3 Abraham Four-Vector of Radiation Reaction

To cancel the rest-mass changing radiation effect, one suspects that also the attached self-field of the particle will be temporarily distorted during the acceleration process. In the following we represent this extra reaction by the four-vector force $\{\kappa^\mu\}$. To preserve the rest mass of our point particle $\{\kappa^\mu\}$ must satisfy the relation

$$w_\mu \kappa^\mu = -P \quad (7.66)$$

in order to compensate for the rest mass change due to radiation (see (7.65)). When we place the particle in an external electromagnetic field, given in terms of the four-force vector $\{F_{\text{ext}}^\mu\} = \gamma(\boldsymbol{\beta} \cdot \mathbf{F}^{\text{ext}}, \mathbf{F}^{\text{ext}})$, where $\mathbf{F}^{\text{ext}}$ is the Newtonian Lorentz force (7.2), the relativistic equation for the μ th component of the particle's four-velocity takes the tentative form

$$m \frac{dw^\mu}{d\tau} = F_{\text{ext}}^\mu - \frac{P}{c_0^2} w^\mu + \kappa^\mu. \quad (7.67)$$

It is possible to obtain an explicit expression for κ^μ by a comparison of (7.49) and (7.66). Equation (7.49) contains the scalar product $\dot{w}_\mu \dot{w}^\mu$ (the dot here means differentiation with respect to the proper time). Differentiation of $w_\mu w^\mu = -c_0^2$ gives $\dot{w}_\mu w^\mu + w_\mu \dot{w}^\mu = 0$ or equivalently $w_\mu \dot{w}^\mu = 0$, since $\dot{w}_\mu w^\mu = w_\mu \dot{w}^\mu$. A second differentiation next gives $w_\mu \ddot{w}^\mu + \dot{w}_\mu \dot{w}^\mu = 0$. The product $\dot{w}_\mu \dot{w}^\mu$ in (7.49) can therefore be replaced by $-w_\mu \ddot{w}^\mu$, and a comparison of the new (7.49) with (7.66) therefore results in

$$\kappa^\mu = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0^3} \frac{d^2 w^\mu}{d\tau^2}. \quad (7.68)$$

By combining (7.67) and (7.68) one obtains the following manifestly covariant equation of motion

$$m \frac{dw^\mu}{d\tau} = F_{\text{ext}}^\mu + \Gamma^\mu, \quad (7.69)$$

with

$$\Gamma^\mu = \frac{1}{4\pi\epsilon_0} \frac{2Q^2}{3c_0^3} \left(\frac{d^2 w^\mu}{d\tau^2} - \frac{dw_\nu}{d\tau} \frac{dw^\nu}{d\tau} w^\mu \right). \quad (7.70)$$

The quantity in (7.70) is the μ th component of what historically is called the Abraham four-vector of radiation reaction [168], and (7.69) is the relativistic Lorentz–Dirac equation [143]. As such this equation is exactly the relativistic generalization of the Abraham–Lorentz equation.

7.3.4 Lorentz–Dirac Equation on Integro-Differential Form

If one writes the Lorentz–Dirac equation in (7.69) in the form (dot stands as before for differentiation with respect to the proper time)

$$m(\dot{w}^\mu - \tau_0 \ddot{w}^\mu) = \Lambda^\mu, \quad (7.71)$$

where

$$\Lambda^\mu = F_{\text{ext}}^\mu - \frac{m\tau_0}{c_0^2} a_\nu a^\nu w^\mu, \quad (7.72)$$

and τ_0 is the characteristic time, given in (7.14), the same integration technique as used in Sect. 7.1 for the nonrelativistic Abraham–Lorentz equation allows us to bring (7.71) into the integral form

$$ma^\mu(\tau) = \int_0^\infty e^{-\alpha} \Lambda^\mu(\tau + \alpha\tau_0) d\alpha. \quad (7.73)$$

This equation is a second-order integro-differential equation for the μ th component of the position four-vector $x^\mu(\tau)$. The integro-differential equations for the four μ -components are coupled through the $a_\nu a^\nu$ -term in (7.72). In the nonrelativistic regime, the equation of motions for three components of $\mathbf{r} = \mathbf{r}(t)$ are much easier to solve (numerically) because only the components of the external force appears under the integral signs; see (7.19). The integro-differential equation in (7.73) must be accompanied by the asymptotic condition

$$\lim_{|\tau| \rightarrow \infty} a^\mu(\tau) = 0. \quad (7.74)$$

Together, (7.73) and (7.74) constitute the relativistic equation of motion for a charged point-particle.

It is possible to establish an integral equation for the acceleration a^μ by contract of the Lorentz–Dirac equation with the covariant acceleration a_μ . Thus,

$$m(a_\mu a^\mu - \tau_0 a_\mu \dot{a}^\mu) = a_\mu F_{\text{ext}}^\mu - \frac{m\tau_0}{c_0^2} a_\nu a^\nu a_\mu w^\mu. \quad (7.75)$$

The condition for rest-mass preservation $ma_\mu w^\mu = 0$ (7.64) eliminates the last term in (7.75), and the relation

$$a_\mu \dot{a}^\mu = \frac{1}{2} \frac{d}{d\tau} (a_\mu a^\mu) \quad (7.76)$$

thereafter leads to

$$m \left[a_\mu a^\mu - \frac{\tau_0}{2} \frac{d}{d\tau} (a_\mu a^\mu) \right] = a_\mu F_{\text{ext}}^\mu. \quad (7.77)$$

This equation is form-identical to (7.71), and the acceleration, therefore, satisfies the integral equation

$$ma_\mu(\tau)a^\mu(\tau) = \int_0^\infty e^{-\alpha} a_\mu(\tau + \frac{1}{2}\tau_0\alpha) F_{\text{ext}}^\mu(\tau + \frac{1}{2}\tau_0\alpha) d\alpha. \quad (7.78)$$

Qualitatively, the relativistic preacceleration effect can be studied assuming that the external force acts so shortly that it can be represented by a delta function applied, say, at $\tau = 0$. With $F_{\text{ext}}^\mu(\tau) = A^\mu \delta(\tau)$, $A^\mu > 0$, the reader may show that (7.78) is reduced to

$$a_\mu(\tau)a^\mu(\tau) = \frac{2}{m\tau_0} a_\mu(0) A^\mu \exp\left(\frac{2\tau}{\tau_0}\right) \theta(-\tau), \quad (7.79)$$

where θ is the Heaviside step function. As expected, the preacceleration appears in the short time interval $-\tau_0 \lesssim \tau \leq 0$ prior to the application of the external delta-function force at $\tau = 0$. For $\tau > 0$, $a^\mu(\tau) = 0$. For a constant force of finite (long) duration a preacceleration effect occurs at the leading edge of the pulse, and a predeceleration effect at the trailing edge. The predeceleration effect can be studied on the basis of (7.79) choosing $A^\mu < 0$.

The term containing $\ddot{w}^\mu$ in the Abraham four-vector of radiation reaction is called the *Schott term* [130, 169]. It is the term by which Γ^μ differs from the radiation reaction force. If the Schott force (7.68) is neglected the Lorentz–Dirac integro-differential equation in (7.73) is reduced to the local form

$$ma^\mu(\tau) = \Lambda^\mu(\tau). \quad (7.80)$$

Since the Schott term is needed to preserve the rest mass, this term does not occur in the nonrelativistic limit, and for $\gamma \rightarrow 1$ the $\mu = 1, 2$ and 3-components of (7.80) become identical to those of the nonrelativistic Newton–Lorentz equation in (7.13).

7.4 Self-Field Distortions

An unaccelerated charged point-particle must carry along its velocity field ((2.61) and (2.67)), and in the particle’s rest frame the attached field is just the electrostatic Coulomb field. This field contains energy, relativistically equivalent to some mass. The Coulomb field energy in space outside a sphere centered on the particle and with radius a is $W^{(0)} = (4\pi\epsilon_0)^{-1} Q^2/(2a)$, where Q is the charge of the particle. The entire electrostatic energy obtained in the limit $a \rightarrow 0$ diverges, $W^{(0)} \rightarrow \infty$, and in consequence the Coulomb field would give an infinite contribution to the rest mass. In the context of near-field optics, the charged “point-particles” are often mesoscopic objects or microscopic ions, and in such cases the internal structure of the particle (object) would show up below a certain radius a_0 . The field energy in space outside the sphere of radius a_0 is finite, and to determine the now finite field

energy inside the object quantum physics is required. For an object of rest mass M quantum mechanics is needed when relevant distances of the order of the de Broglie wavelength appear, and field theory is necessary when distances of the order of the Compton wavelength

$$\lambda_C = \frac{h}{Mc_0} \quad (7.81)$$

are reached. The wavelength λ_C originates in Compton's famous quantum theory for scattering of X-rays by electrons [170]. In this work he assumed that the X-ray beam consisted of localized quanta. An almost identical explanation for the observed wavelength shift of the rays was given simultaneously and independently by Debye [171]. When near-field optical problems are studied on the basis of quantum mechanics infinite self-energies do not occur, and the distances of interest are always much larger than the Compton wavelength. If one assumes (incorrectly) that the electron ($Q = -e$, $M = m_{\text{em}}$) is a purely electromagnetic and spherical object of classical (cl) radius (R^{cl}), and with its charge distributed uniformly over the surface of the sphere (this makes the field vanish inside the sphere), the electromagnetic (em) rest mass will be given by

$$m_{\text{em}} = \frac{W^{(0)}}{c_0^2}. \quad (7.82)$$

Within an unimportant factor of 2, (7.82) leads to the expression given in (7.25) for the classical radius of the electron (setting $m = m_{\text{em}}$). The classical electron radius is ≈ 137 times smaller than the electron Compton wavelength (divided by 2π),

$$\frac{\hbar}{m_{\text{em}}c_0} = \frac{4\pi\epsilon_0\hbar c_0}{e^2} \frac{e^2}{4\pi\epsilon_0 m_{\text{em}}c_0^2}, \quad (7.83)$$

and at such distances quantum field phenomena are important since interaction energies of the order $e^2/(4\pi\epsilon_0 R^{\text{cl}}) = m_{\text{em}}c_0^2$ occur. A rigorous quantum field-theoretical description is needed then. The observed (experimental) mass of the electron

$$m = m_{\text{bare}} + m_{\text{em}} \quad (7.84)$$

deviates from the electromagnetic by an amount one might call the bare (or field-undressed) mass. An understanding of the structure of elementary point particles (their mass, charge,...) such as electrons, muons and quarks lies totally outside the domain of classical physics, and in the framework of microscopic classical electrodynamics with point particles the experimental mass of the electron must be fed in as a phenomenological quantity, determined experimentally.

Observed from an inertial frame moving with respect to the rest frame of the point-particle the attached self-energy $W^{(0)}$ will be given by $W = \gamma W^{(0)}$ where the particle velocity $\mathbf{v} = c_0\boldsymbol{\beta}$ in the new frame appears in the γ -factor. In the rest frame the particle's electromagnetic momentum is zero (as is the total momentum) but in the new frame the velocity field contributes a momentum

$$\frac{W}{c_0^2} \mathbf{v} = \frac{\gamma W^{(0)} \boldsymbol{\beta}}{c_0} \quad (7.85)$$

to the uniformly moving particle.

When the particle is accelerated temporary distortions in the electromagnetic self-energy and self-momentum must occur to preserve the structureless particle's rest mass during the Larmor–Lienard emission of radiative field energy and momentum. A qualitative discussion of the self-energy distortions can be given on the basis of the $\mu = 0$ -component of the Lorentz–Dirac equation. If the external Newtonian force is denoted by $\mathcal{F}^{\text{ext}}$ and we introduce $\mathbf{w} = \gamma \mathbf{v} = \gamma d\mathbf{r}/dt = d\mathbf{r}/d\tau$ one obtains

$$\frac{dE^{\text{dyn}}(\tau)}{d\tau} = \mathbf{w} \cdot \mathcal{F}^{\text{ext}} - \gamma P, \quad (7.86)$$

where

$$E^{\text{dyn}}(\tau) = \left(\gamma - \tau_0 \frac{d\gamma}{d\tau} \right) mc_0^2. \quad (7.87)$$

It appears from (7.86) that the quantity $E^{\text{dyn}}(\tau)$ may be considered as the instantaneous dynamic (dyn) self-energy of the particle, since the rate of change per unit proper time equals the rate of work carried out by the external force on the particle ($\mathbf{w} \cdot \mathcal{F}^{\text{ext}}$) minus the rate of radiative energy loss per unit proper time. The dynamic self-energy deviates from the attached self-energy, $\gamma(\tau)mc_0^2$, of a particle moving uniformly with the (instantaneous) velocity $\mathbf{v}$, by the Schott term

$$\tau_0 \frac{d\gamma}{d\tau} mc_0^2 = \gamma^2 \tau_0 \boldsymbol{\beta} \cdot \frac{d\boldsymbol{\beta}}{d\tau} (\gamma mc_0^2). \quad (7.88)$$

At instants of positive acceleration parallel to the velocity [$\boldsymbol{\beta} \cdot d\boldsymbol{\beta}/d\tau > 0$] the dynamic self-energy is less than γmc_0^2 , and for negative acceleration parallel to $\mathbf{v}$, $E^{\text{dyn}} > \gamma mc_0^2$. The deviation of the dynamic mass from γmc_0^2 can be understood as a result of the fact that parts of the electromagnetic rest mass – spread out over the region of the Coulomb field – cannot acquire the velocity change (positive or negative) of the charged particle “itself” until all of it is reached by a light signal propagating with the finite speed c_0 . The self-energy distortion is a near-field effect in the sense that it only takes place in the r^{-2} -zone around the point particle. In the nonrelativistic domain, self-field distortions do not occur.

The distortion in the self-momentum during accelerated particle motion can be studied via the $\mu = 1, 2, 3$ -components of the Lorentz–Dirac equation. As we shall realize in Part II of this book, the divergence-free part of an external vector potential, $\mathbf{A}_T^{\text{ext}}(\mathbf{r}, t)$, adds a momentum $Q \mathbf{A}_T^{\text{ext}}(\mathbf{r}_Q(t), t)$ to the point particle located at $\mathbf{r}_Q = \mathbf{r}_Q(t)$ at time t . The field momentum attached to the moving particle spreads over the Coulomb self-field region, and as soon as the magnetic field of the external source, $\mathbf{B}^{\text{ext}}$, overlaps this region the attached field momentum starts to be distorted. The dynamic self-momentum of an accelerated point particle, therefore, deviates from the self-momentum of a uniformly moving particle in accordance with what appears from an analysis of the Scott term in the Lorentz–Dirac equation.

Part II
Quantum Theory with Classical Fields

Chapter 8

About Local-Field Theory Based on Electron–Photon Wave Mechanics

It appears from the description in various chapters of Part I that the local-field concept plays a central role in near-field and mesoscopic electrodynamics. Since the local fields vary considerably on the atomic length scale studies of the particle dynamics cannot be based on the Newton–Lorentz equation, as it was done originally by Lorentz [138, 172] in his ambitious program of “separating matter and aether” [18, 27, 173]. By replacing Newtonian mechanics by its nonclassical covering theory, i.e., nonrelativistic wave mechanics, one obtains a satisfactory starting point for most theoretical studies in near-field and mesoscopic electrodynamics. Many aspects of local-field electrodynamics are covered in the reviews by Cho [174], Stahl and Balslev [175], and the present author [5, 49]. In a few cases it may be necessary also to replace Newtonian mechanics by its classical covering, viz., relativistic mechanics. This will be the case, for instance, when a relativistic particle moves parallel to a surface in the evanescent tail of a surface wave or penetrates a condensed-matter medium. Relativistic aspects of local-field electrodynamics can be of importance in microscopic response theory. Thus, when an object under study moves with respect to the source exciting the object (or/and the detector receiving the object response) it may be necessary to make an inertial-frame independent calculation of the microscopic response function of the object, *even* if the relative velocity of object and source (detector) is small. The relativistic wave mechanics of massive particles (electrons) is of interest in near-field studies where the electron spin dynamics plays a role. Although it in most cases is sufficient to base the practical calculations on the weakly-relativistic Pauli equation, it might be necessary for a fundamental understanding to start from the fully-relativistic Dirac equation. The spatial localization problem for photons cannot, at least from my standpoint, be fully explored without involving the field–matter interaction. In fact, I have argued on several occasions that it is the Compton wavelength of the *electron* which sets the fundamental limit for how strongly localized a photon can be prepared in space; see e.g., [176].

In Part II of this book, we base our studies on the so-called semiclassical theory of electrodynamics, a theory in which the electrons (massive particles) are treated quantum mechanically and the electromagnetic field classically. Quantum optics, the covering theory of classical electromagnetic field theory, has become of increasing importance in near-field electrodynamics in recent years, and in Part III, the

second-quantized field formalism will be used to investigate a number of physical phenomena of interest in near-field quantum electrodynamics.

Although the studies in Part II is based on microscopic classical field theory, we reformulate this theory in such a manner that it appears as a first-quantized theory for photons, i.e., what is called photon wave mechanics. Although all results obtained starting from photon wave mechanics for a single photon are physically equivalent to those obtained via the classical field theory, the wave mechanical picture enables us to see many subjects in a new perspective. This, in itself makes the study and use of photon wave mechanics useful. Moreover, calculational techniques known from electron wave mechanics can be transferred to photon wave mechanics, and thereby provide us with new tools for studies of the semiclassical field–matter interaction. Also, it seems to me that the rather unknown theory of photon wave mechanics deserves to be better known among physicists. Photon wave mechanics also helps us a bit in achieving a unified description of all elementary particles.

8.1 Dynamical Variables and Redundancy: Rim Zone

In special relativity, inertial systems play a prominent role, and an essential distinction must be made between uniform and nonuniform particle motion relative to a given inertial frame. In electrodynamics, the distinction appears in the form of velocity fields and acceleration fields [19, 116, 130]. The last type of fields, also called radiation fields, are emitted only if the charged particle is moving nonuniformly. The separation into velocity and acceleration fields is obviously convenient in electrodynamic investigations where it is important to retain manifest covariance in the various steps of the calculation. In near-field electrodynamics, a different separation of the electromagnetic field is instructive, namely the less common separation into solenoidal and irrotational fields [5, 49, 119, 126, 130]. Although this separation is not frame independent, nor commonly used in the near-field community, I argue in some detail for its value in near-field electrodynamics in Chap. 9. It may be useful here to highlight a few points.

A solenoidal *vector field* is defined as one which is divergence-free (often called just transverse (T)) *everywhere in space*. It appears from one of the Maxwell–Lorentz equations that the electric field ($\mathbf{E}$) outside a continuous (in the quantum mechanical sense probabilistic) charge density distribution has a vanishing divergence, i.e., $\nabla \cdot \mathbf{E} = 0$, but this does not imply that $\mathbf{E}$ here is a divergence-free *vector-field*. Close to matter, in a zone I have called the rim zone [177], one also has $\nabla \times \mathbf{E} = \mathbf{0}$. In the rim zone the electric field is *both* divergence-free and rotational-free (also called longitudinal (L)) *but not identically zero*. The rim zone hence is characterized by the criterion

$$\nabla \cdot \mathbf{E}_L(\mathbf{r}, t) = 0, \quad (8.1)$$

where $\mathbf{E}_L (\neq \mathbf{0})$ is the longitudinal part of the electric field. Although the new sub-field of physical optics, called near-field optics has emerged over the last quarter

of a century or so, a survey of the literature shows that what is meant by the word “near” in near-field optics has never been properly defined. Recently, I have suggested that physics in the rim zone is near-field optics, or in a broader context near-field electrodynamics.

A division of the Maxwell–Lorentz equations into their transverse and longitudinal vector field parts leads to the result that the longitudinal electric field equals the instantaneous Coulomb field of an assembly of point-particles. Since the Coulomb field can be expressed exclusively in terms of the particle position coordinates, the global state of a coupled field–matter system at a given time is completely specified giving the magnetic field and the transverse part of the electric field in every space point, plus the position and velocity variables of all particles [178]. This fact is of crucial importance for the quantization scheme leading up to the (transverse) photon concept. The elimination of the longitudinal electric field in favor of the particle position coordinates removes an otherwise existent redundancy in the description of electrodynamics.

The fact that the transverse part of the electric vector field is related in a *spatially nonlocal* manner to the total electric field has the consequence that a photon emitted from matter in the initial phase is no better localized in space than the rim zone volume [108, 109, 179, 180].

The longitudinal field in combination with the magnetic field give a contribution to what at first may be called the field momentum. Since this contribution can be expressed solely in terms of the transverse part of the vector potential (A_T) in the various particle positions, the total (generalized) momentum of a particle (charge q) takes the form [178]

$$\mathbf{p} = \boldsymbol{\pi} + q\mathbf{A}_T, \quad (8.2)$$

where $\boldsymbol{\pi}$ is the (relativistic) mechanical momentum of the particle. The generalized momentum ($\mathbf{p}$) in quantum mechanics is identified with the particle canonical momentum which translates into a momentum operator. The consistency of the result in (8.2) is underlined by the fact that the transverse part of a vector potential is gauge invariant.

8.2 Linear Response Theory in a Microscopic Perspective

Notwithstanding obvious shortcomings, calculations in near-field electrodynamics often are based on a combination of the macroscopic Maxwell equations (given in (1.1)–(1.4)) and constitutive relations ((1.5)–(1.7)) of some specified form [23–25, 181–189]. If the field–matter interaction is sufficiently weak, the constitutive relations take well-known linear forms. With a view to later microscopic considerations, it is useful to write the right hand side of (1.3) as a generalized current density, $\langle \mathbf{J} \rangle_{\text{gen}}$, so that

$$\langle \mathbf{J} \rangle_{\text{gen}}(\omega) = \langle \mathbf{J} \rangle(\omega) - i\omega \langle \mathbf{D} \rangle(\omega) \quad (8.3)$$

in the frequency domain. In the linear regime, one takes $\langle \mathbf{J} \rangle(\omega) = \boldsymbol{\sigma}(\omega) \cdot \langle \mathbf{E} \rangle(\omega)$, $\langle \mathbf{D} \rangle(\omega) = \epsilon_0 \boldsymbol{\epsilon}(\omega) \cdot \langle \mathbf{E} \rangle(\omega)$, and $\langle \mathbf{J} \rangle_{\text{gen}}(\omega) = \boldsymbol{\sigma}_{\text{gen}}(\omega) \cdot \langle \mathbf{E} \rangle(\omega)$, with the result

$$\boldsymbol{\sigma}_{\text{gen}}(\omega) = \boldsymbol{\sigma}(\omega) - i\epsilon_0\omega\boldsymbol{\epsilon}(\omega). \quad (8.4)$$

The generalized macroscopic conductivity tensor, $\boldsymbol{\sigma}_{\text{gen}}(\omega)$, thus combines the conductivity response of the “free” electrons (via $\boldsymbol{\sigma}(\omega)$) and the dielectric response of the “bound” electrons (via $\boldsymbol{\epsilon}(\omega)$). For brevity, we omit the subscript “gen” in the following, that is $\langle \mathbf{J} \rangle_{\text{gen}} \equiv \langle \mathbf{J} \rangle$ and $\boldsymbol{\sigma}_{\text{gen}} \equiv \boldsymbol{\sigma}$. Transformed to the time domain, the generalized macroscopic constitutive relation $\langle \mathbf{J} \rangle(\omega) = \boldsymbol{\sigma}(\omega) \cdot \langle \mathbf{E} \rangle(\omega)$ takes the form

$$\langle \mathbf{J} \rangle(t) = (2\pi)^{-1} \int_{-\infty}^{\infty} \boldsymbol{\sigma}(t - t') \cdot \langle \mathbf{E} \rangle(t') dt'. \quad (8.5)$$

Frequency dispersion in $\boldsymbol{\sigma}(\omega)$ thus means that the relation between $\langle \mathbf{J} \rangle(t)$ and $\langle \mathbf{E} \rangle(t)$ is nonlocal in time. To use a $\boldsymbol{\sigma}(\omega)$ it is necessary that the macroscopic physical properties of the medium exhibit infinitesimal translational invariance in time (are time independent). If the medium changes its properties over time, the conductivity would depend on both times t and t' , separately, and not only on their difference. Transformed to the Fourier domain $\boldsymbol{\sigma}(t, t')$ would be a function of two frequencies, i.e., $\boldsymbol{\sigma}(\omega, \omega')$. If the medium is inhomogeneous on a macroscopic length scale the conductivity is space ($\mathbf{r}$)-dependent, i.e., $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{r}; \omega)$.

In the Maxwell–Lorentz theory, only microscopic current and charge densities appear, and the local electromagnetic fields vary rapidly in space (and time). The linear constitutive equation, which relates the microscopic current density, $\mathbf{J}(\mathbf{r}; \omega)$, to the local electric field, $\mathbf{E}(\mathbf{r}; \omega)$, has the spatially nonlocal form [21, 118, 190–196]

$$\mathbf{J}(\mathbf{r}; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}(\mathbf{r}'; \omega) d^3 r', \quad (8.6)$$

provided we uphold the translational invariance in time, a strong limitation, yet of no importance in what follows. For an extension to nonlinear electrodynamics see [197], and references herein. Quantum mechanics (and in fact also Newtonian mechanics) basically always leads to a spatially nonlocal relation between $\mathbf{J}(\mathbf{r}; \omega)$ and $\mathbf{E}(\mathbf{r}; \omega)$, and in the context of near-field electrodynamics where one necessarily must treat physical properties on a subwavelength scale, the two-point $(\mathbf{r}, \mathbf{r}')$ dependence of the microscopic conductivity tensor, $\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega)$, indicated in (8.6), often is indispensable. Infinitesimal translational invariance in space, which never occurs exactly on a microscopic scale, would replace $\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ by $\boldsymbol{\sigma}(\mathbf{r} - \mathbf{r}'; \omega)$. A spatial Fourier transform then would lead to the algebraic relation

$$\mathbf{J}(\mathbf{q}, \omega) = \boldsymbol{\sigma}(\mathbf{q}, \omega) \cdot \mathbf{E}(\mathbf{q}, \omega). \quad (8.7)$$

When the spatial nonlocality takes the form given by (8.7) one often use the name *spatial dispersion* [21, 22, 85, 118, 198–203]. There are situations in physics, where the approximate connection in (8.7) may be used. A prominent example is

BCS-superconductivity, where the infinite electrical conductivity at $\omega = 0$ is hidden in $\lim_{\omega \rightarrow 0} \sigma(\mathbf{q} = 0, \omega)$, and the Meisner effect derives from $\lim_{\mathbf{q} \rightarrow 0} \sigma(\mathbf{q}, \omega = 0)$ [98, 200]. From a relativistic point of view the form $\sigma(\mathbf{q}, \omega)$ has some interest because $(\omega/c_0, \mathbf{q})$ constitutes a four-vector. An assumption of *finite* translational invariance in space is often inadequate in studies of the electrodynamic properties of solids which exhibit lattice periodicity in the bulk. Starting from the level of sophistication given in (8.6), I shall in Chap. 10 develop the linear microscopic response theory further, discussing among other aspects those mentioned below.

The discussion of dynamical variables and redundancy in Sect. 8.1 indicates that the longitudinal part of the electrical field is taken account of once the Schrödinger equation (or the Dirac equation) is used to calculate $\sigma(\mathbf{r}, \mathbf{r}'; \omega)$. In microscopic response theory, the driving field thus is the transverse part $\mathbf{E}_T(\mathbf{r}; \omega)$ of the local electric field. In the constitutive relation (8.6), the old conductivity ($\sigma(\mathbf{r}, \mathbf{r}'; \omega)$) is thus replaced by a new one ($\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$), and instead of $\mathbf{E}(\mathbf{r}'; \omega)$ now $\mathbf{E}_T(\mathbf{r}'; \omega)$ appears.

As the word *response* indicates something must *respond* to a *cause*. To throw light on this, we consider two groups of charged particles separated so far from each other that their rim zones do not overlap (effectively). For explicable reasons, the groups are referred to as source and system. The current density distribution in the source gives rise to a so-called external field in the surroundings, and the transverse part of this, $\mathbf{E}_T^{\text{ext}}$, acts with some time delay on the system particles. In response theory, $\mathbf{E}_T^{\text{ext}}$ is the *cause* of the induced current density *response*, $\mathbf{J}$, of the system. When the system particles are set in motion they themselves generate an electric field which, when calculated selfconsistently and added to the external field, gives us the local field. The transverse part of this is the $\mathbf{E}_T$ mentioned above. As we shall realize in Chap. 10, it is possible to eliminate (at least in principle) $\mathbf{E}_T$ in favor of $\mathbf{E}_T^{\text{ext}}$ in the microscopic constitutive relation. With this done, and the *new* conductivity tensor denoted by σ , we finally arrive at the *causal* constitutive relation

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \sigma(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3r' \quad (8.8)$$

in the space–time domain.

The relation between $\mathbf{J}$ and $\mathbf{E}_T^{\text{ext}}$ is causal in the sense that there can be no induced current density in a given point *before* the external field is applied. Mathematically, this form of causality is expressed through the fact that σ is zero for $t' > t$ (independent of $\mathbf{r}$ and $\mathbf{r}'$). In contrast, the relation between $\mathbf{J}$ and $\mathbf{E}_T$, and between $\mathbf{J}$ and $\mathbf{E}$, is not causal. The nonlocal connection between the transverse fields $\mathbf{E}_T$ and $\mathbf{E}_T^{\text{ext}}$ is of course also causal.

Causality, i.e., here the absence of advanced effects in physics, leads to the existence of certain general frequency dispersion relations in linear response theory. Such dispersion relations, which often are named Kramers–Kronig relations [22, 199, 200, 203–205], are integral relations between the real and imaginary parts of all causal response functions in the frequency domain, e.g., the microscopic conductivity tensor in (8.8). Although the correct use of the Kramers–Kronig relations

requires causality, one often sees them applied in an uncritical manner in the literature. For instance, it is not uncommon to see them applied to the dielectric function $\epsilon(\omega)$ relating the displacement field $\langle \mathbf{D} \rangle(\omega)$ to the *selfconsistent* field $\langle \mathbf{E} \rangle(\omega)$ in macroscopic electrodynamics.

When spatially nonlocal effects are of importance, as they most often are in near-field and mesoscopic electrodynamics, great care must be taken in the introduction of microscopic “polarization ($\mathbf{P}$)” and “magnetization ($\mathbf{M}$)” concepts. Part of the complication stems from the fact that the $\mathbf{P}$ - and $\mathbf{M}$ -fields only enter microscopic physics in a combination of derivatives, viz.,

$$\frac{\partial \mathbf{P}}{\partial t} + \nabla \times \mathbf{M} = \mathbf{J}, \quad (8.9)$$

where $\mathbf{J}$ is the microscopic current density appearing in the Maxwell–Lorentz theory. The flexibility in our choice of $\mathbf{P}$ and $\mathbf{M}$, has the consequence that linear constitutive relations can be set up in various manners, which all end up with the same physical conclusions regarding observations. In nonlocal electrodynamics, all “magnetic” effects, usually described via a *generalized* magnetic permeability (μ) can thus be included in the *generalized* electric permittivity (ϵ) [118, 119]. For media exhibiting (approximately) translational invariance in space–time, and with the extension of the theory from $\epsilon(\omega)$ to $\epsilon(\mathbf{q}, \omega)$, i.e., from locality to nonlocality in space, all magnetic effects may be incorporated in the $\mathbf{q}$ -dependence of ϵ . At first sight this may come as a surprise to the reader, but in Chap. 10 we shall understand the reason behind this fact.

8.3 On the Quantum Mechanical Calculation of Microscopic Conductivity Tensors

In the semiclassical theory of electrodynamics, the current density $\mathbf{J}(\mathbf{r}, t)$ appearing in the microscopic Maxwell–Lorentz equations is identified with an appropriate mean value of the current density operator $\hat{\mathbf{j}}(\mathbf{r}, t)$ of the particles [5, 49, 206–212]. The mean value is conveniently calculated by means of the density matrix (operator) formalism described in Sects. 11.1 and 11.2. The density matrix operator satisfies the quantum mechanical Liouville equation, which in a certain sense can be considered as an extension of the Boltzmann equation known from classical statistical mechanics. It is necessary to deal with the quantum dynamics of statistical mixtures of states, because, already before we excite the particles by some electromagnetic field, our knowledge of the state of the quantum system is incomplete. Typically, one starts with a particle system in thermal equilibrium. In order to determine the density matrix belonging to a statistical mixture from the Liouville equation one must know the relevant Hamilton operator for the system. In this book we begin from a study of the relativistic standard Hamiltonian, and the heuristic extension needed in the classical framework to reach the weakly relativistic Pauli Hamiltonian. The

usual canonical quantization procedure then leads us to the minimal coupling form of the relativistic (or nonrelativistic) Hamilton operator for a system of spinless particles. In order to quantize the Pauli Hamiltonian, one also needs to quantize the spin angular momentum of the electron. This is done using the standard procedure for quantization of angular momenta.

The orbital probability current density of a nonrelativistic particle is divided into two parts, viz., (1) a part which can be written as a certain bilinear combination of the particle wave function and its spatial gradient and (2) a part, which depends explicitly on the local vector potential. Only the sum of the two parts is gauge invariant. If only the transverse part of the vector potential is kept in the last part, and the rest transferred to the first part, a division into two parts which both are gauge invariants results. The two new parts are the so-called paramagnetic and diamagnetic probability current densities.

The mean value of the current density operator is calculated from

$$\mathbf{J}(\mathbf{r}, t) = \text{Tr}\{\hat{\rho}\hat{\mathbf{j}}\}, \quad (8.10)$$

where $\hat{\rho}$ is the density matrix operator of the system, and in a weak external electromagnetic field it turns out that $\mathbf{J}(\mathbf{r}; \omega)$ is related in a linear, yet spatially nonlocal, manner to the sum of the transverse part of the local electric field and the longitudinal part of the external electric field. The generalized response tensor $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ which emerges has the same *formal structure* in the single- and many-body approaches.

The $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ -tensor consists of a spatially nonlocal paramagnetic part and a spatially local diamagnetic part, and each part diverges in the low-frequency ($\omega \rightarrow 0$) limit. By rewriting the diamagnetic part of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ in an *apparently* nonlocal form [49], it is shown (Sect. 12.3) that the sum of the two parts remains finite for $\omega \rightarrow 0$. Although quantum electrodynamics as such is a gauge invariant theory, it is certainly not obvious that the linearization of the current density response results in a gauge invariant expression for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$. It is shown (Sect. 12.4) by a direct calculation that the linear response *is* gauge invariant, however. Such a result, which holds both in a single-electron [209] and in a many-electron [5] approach, is important for fundamental studies of local-field effects in mesoscopic optics and near-field electrodynamics.

8.4 Coupled-Antenna Theory

From a knowledge of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ it is not difficult to obtain the microscopic quantum mechanical expression for the linear response tensor $\mathbf{S}_{\text{TT}}(\mathbf{r}, \mathbf{r}'; \omega)$ which, in a spatially nonlocal manner, relates the transverse parts of the current density and the local electric field. From a physical point of view, $\mathbf{S}_{\text{TT}}(\mathbf{r}, \mathbf{r}'; \omega)$ has a beautiful simple structure, as I now shall indicate. Thus, each quantum transition between two stationary many-body states gives its own contribution to $\mathbf{S}_{\text{TT}}(\mathbf{r}, \mathbf{r}'; \omega)$. The

tensorial form of a given contribution, say between the quantum states K and L , is given by a dyadic product $\mathbf{j}_{K \rightarrow L}^T(\mathbf{r})\mathbf{j}_{L \rightarrow K}^T(\mathbf{r}')$. The quantity $\mathbf{j}_{K \rightarrow L}(\mathbf{j}_{L \rightarrow K})$ is the transition current density *from* state K (L) *to* state L (K) and the added superscript T means that the transverse vector field part $\mathbf{j}_{K \rightarrow L}^T(\mathbf{j}_{L \rightarrow K}^T)$ of $\mathbf{j}_{K \rightarrow L}(\mathbf{j}_{L \rightarrow K})$ enters the description. In the $L \rightarrow K$ transition the rate of work carried out locally (at $\mathbf{r}'$) by the transverse part of the local field, $\mathbf{E}_T(\mathbf{r}'; \omega)$, will be proportional to $\mathbf{j}_{L \rightarrow K}^T(\mathbf{r}') \cdot \mathbf{E}_T(\mathbf{r}'; \omega)$. Integration of this product over $\mathbf{r}'$ -space gives a quantity proportional to the entire work. In the return process, $K \rightarrow L$, $\mathbf{j}_{K \rightarrow L}^T(\mathbf{r})$ serves as the source current density distribution for the emitted electric field. Field emission takes place from the entire rim zone, and the Huygens scalar propagator describes how the field develops in space–time.

A microscopic version of the classical Ewald–Oseen extinction theorem is used to establish an integral relation between the transverse parts, $\mathbf{E}_T(\mathbf{r}; \omega)$ and $\mathbf{J}_T(\mathbf{r}'; \omega)$, of the local field and the quantum mechanical mean value of the current density operator of the particle system. The constitutive relation between $\mathbf{J}_T$ and $\mathbf{E}_T$, finally leads to an integral equation for the transverse part of the local field. The integral equation problem can be transferred to a matrix equation problem without discretization in space because the kernel associated with a given transition is separable, cf. the dyadic form $\mathbf{j}_{K \rightarrow L}^T(\mathbf{r})\mathbf{j}_{L \rightarrow K}^T(\mathbf{r}')$ [5, 49]. Once transferred to a matrix problem, the microscopic criterion for local-field resonance can be derived without difficulty.

8.5 Electromagnetic Propagators and Nonretarded Transverse Response

Electromagnetic Green functions and propagators play a prominent role in near-field electrodynamics, and in Chap. 14 we follow-up on the analysis presented in Chap. 3. The standard Green function for the electric field does not vanish in the nonretarded limit, i.e., for $c_0 \rightarrow \infty$ (formally). By proper subtraction of the nonretarded part from $\mathbf{G}(\mathbf{R}; \omega)$, one obtains a genuine transverse propagator $\mathbf{G}_T(\mathbf{R}; \omega)$ which Fourier transform does exist. Without going into details let us take a glance at the form $\mathbf{G}_T$ takes in the space–time domain. Here [49–51],

$$\begin{aligned} \mathbf{G}_T(\mathbf{R}, \tau) = & \frac{1}{4\pi R} \delta\left(\frac{R}{c_0} - \tau\right) \left(\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}\right) \\ & - \frac{c_0^2 \tau}{4\pi R^3} \theta(\tau) \theta\left(\frac{R}{c_0} - \tau\right) \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}\right). \end{aligned} \quad (8.11)$$

The first term on the right side of this equation is a far-field term, nonvanishing only on the light cone, and the second term is a near-field term. It is remarkable perhaps that there is no mid-field term in (8.11). The step functions in the near-field term show that the field response is causal ($\theta(\tau)$) and space-like ($\theta[(R/c_0) - \tau]$). The

last fact is in no way in conflict with Einsteinian causality because the rim zone is the source region for the transverse field. When the source extension “artificially” is compressed from the $\mathbf{J}_T$ - to the $\mathbf{J}$ -domain, an apparently space-like coupling necessarily emerges in the rim zone domain. The space-like character of the near-field part $\mathbf{G}_T(\mathbf{R}, \tau)$ also ensures that the volume integral of $\mathbf{G}_T \cdot \mathbf{J}$ is absolutely convergent. (In itself, an R^{-3} -singularity would lead to a conditionally convergent integral, a result which from a physical point of view is unacceptable).

Besides the radiative contribution, described via $\mathbf{G}_T(\mathbf{R}, \tau)$, the transverse electric field also has a nonradiative part, but only in the rim zone (and inside the source current density distribution). This nonradiative part of $\mathbf{E}_T$ is of great importance in near-field electrodynamics. Upon an extension of a calculation originally carried out by Yaghjian [45] to the microscopic domain, we study the nonradiative part of $\mathbf{E}_T$ in some detail in Sects. 14.3–14.5. For various purposes in near-field electrodynamics, it is useful to divide the nonradiative contribution to $\mathbf{E}_T$ into spatially nonlocal and local parts. The local component usually is called the transverse self-field term. The balance between the local and nonlocal parts depends on the choice made for the form of the contraction volume used to handle the R^{-3} -singularity, and physically only the sum of the two parts makes sense. In near-field optics, spherical contraction around the singularity most often is employed. In this case, only a self-field term exists.

We finish our examination of the electromagnetic propagator formalism by showing the relativistic covariance of the Huygens propagator. In Chap. 24, we follow-up on this by studies of integral representations for various covariant propagators.

8.6 Photon Wave Mechanics: A Reinterpretation of Maxwells Theory

The Maxwell equations in empty space can be reformulated in such a manner that they appear as a wave mechanical theory for photons. As such, photon wave mechanics can be considered as the first-quantized theory for the photon; see [180, 213], and references in these monographs. Upon second-quantization, the quantum optical level is reached. Although certain aspects of photon wave mechanics date back to around 1930 [214–216], and have been of some interest ever since, the theory still is rather unknown among physicists. However, the photon interpretation helps us to obtain a unified view of all elementary particles in physics, and of importance here, it certainly gives one a new perspective of certain fundamental aspects of near-field electrodynamics. From an observational point of view it is necessary that photon wave mechanics is extended so as to take into account field–matter interactions. In free space photon wave functions can be constructed in various manners, the only demand being that different choices lead to the same observational conclusions in the end.

In Chap. 15, we study photon wave mechanics on the basis of the so-called complex field theory, starting from the original Landau–Peierls theory [214]. Since a

photon necessarily has positive energy, only positive-frequency solutions to the free Maxwell theory enter the photon theory. In consequence, complex analytical signals play a central role in photon wave mechanics. In a classical physical context the analytical signal satisfies a spatially nonlocal first-order differential equation in time [53]. The equation is usually named Sudarshan’s equation referring to Sudarshan’s derivation from 1969 [217]. In fact, the Landau–Peierls equation for the photon wave function established much earlier (in 1930) is form-identical to Sudarshan’s equation.

The complex field theory of the photon takes a particularly nice form in the momentum–time domain, and it accentuates the photon helicity concept. The scalar amplitudes of two complex field vectors, which relate closely to the photon helicity, satisfy form-identical Schrödinger-like wave equations, and may be considered as photon wave functions for the two helicity species. Using these wave functions, the one-photon energy–momentum four-vector appears as the quantum mechanical mean value of a four-momentum operator. In the space–time domain, the wave equations for the two complex field vectors take a suggestive form if one introduces a certain Cartesian photon spin operator. The photon Schrödinger-like wave equations for the complex field vectors both have Hamilton operators proportional to the scalar product between the dimensionless photon spin-1 ($\hat{\mathcal{S}}$) and momentum ($\hat{\mathbf{p}}$) operators. If the photon wave functions of positive and negative helicity are denoted by ψ_+ and ψ_- , respectively, the photon wave equations,

$$i\hbar \frac{\partial}{\partial t} \psi_{\pm} = \pm c_0 (\hat{\mathcal{S}} \cdot \hat{\mathbf{p}}) \psi_{\pm}, \quad (8.12)$$

are form-identical to those of the right-handed screw antineutrino (wave function: ϕ_+) and left-handed screw neutrino (ϕ_-), viz.,

$$i\hbar \frac{\partial}{\partial t} \phi_{\pm} = c_0 (\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{p}}) \phi_{\pm}, \quad (8.13)$$

$\hat{\boldsymbol{\sigma}}$ being the (normalized) Pauli spin operator, appropriate for spin-1/2 particles. A photon probability current density concept can also be introduced in the complex field theory [180], and the concept has much in common with the Cook photon current density which relates to the Mandel–Cook coarse-grained photon localization theory in quantum optics [53, 218–221].

In the complex field theory, there is a spatially nonlocal connection between the electromagnetic field vectors and the photon wave function. Hence, the kernel relating the wave function in a given space point ($\mathbf{r}$) to the field in surrounding points ($\mathbf{r}'$) has a distance dependence proportional to $|\mathbf{r} - \mathbf{r}'|^{-5/2}$. The inverse kernel decays with distance as $|\mathbf{r} - \mathbf{r}'|^{-7/2}$ [180]. For comparison, the rim zone of a point-particle (atom, mesoscopic object) has an extension characterized by the function $|\mathbf{r} - \mathbf{r}'|^{-6/2}$. The spatially nonlocal, but timely local, connection between the electromagnetic field vectors and the photon wave function makes the complex field theory less attractive from a relativistic perspective. Other choices for a photon

wave function formalism, which are quite satisfactory relativistically, are discussed in Chap. 16.

Starting from the Riemann–Silberstein approach to classical electromagnetics in free space [222–224], a so-called photon energy wave function formalism can be set up (see Sects. 16.1–16.3). In this formalism, which has been advocated by Molière [225] and Good [226], and in recent years by Sipe [228], Birula-Bialynichi [213, 227] (and myself [229]), the relation between the photon energy wave function and the field is local in space–time. The addition of the word “energy” between “photon” and “wave function” relates to the circumstance that the photon probability density is just the properly normalized field energy probability. The quantum mechanical value of the photon energy–momentum four-vector operator is obtained from a Lorentz-invariant integration on the light-cone.

An attractive four-potential theory of photon wave mechanics can be established starting from the complex field theory, as we demonstrate in Sect. 16.3. If one in this theory replaces the transverse electric and magnetic fields entering the wave function by their expressions in terms of the *transverse* vector potential, one ends up with what may be called the wave function of a vectorial transverse photon. From this vectorial function two transverse scalar photon wave functions, belonging, e.g., to the two helicity species, can be introduced. Two new types of photon wave functions are then put on the scene by replacing one of the helicity components of the transverse vector potential by (1) the amplitude of the longitudinal part of the vector potential and (2) the scalar potential [180, 230]. The longitudinal and scalar potentials are gauge dependent, and to obtain a covariant photon wave mechanical theory, one chooses the Lorenz gauge. In this gauge, we are led to a four-potential theory with four types of light particles (two transverse, a longitudinal, and a scalar photon). The wave functions of these photon types satisfy form-identical Schrödinger-like equations.

8.7 Near-Field and Gauge Photons: Photon Embryo

In high-energy physics, it is often convenient, and sometimes even necessary, to carry out quantum electrodynamic analyses in such a manner that the Lorentz covariance is manifest throughout the calculations [117, 154, 156, 178]. In case, the starting point is the extension of the four photon theory described above to the field-quantized level. In low-energy physics, the covariant theory is seldom used. Instead, one chooses the Coulomb gauge, which explicitly yields the Coulomb interaction between the various particles [178]. At low energies this interaction usually is the strongest, and the Coulomb gauge gives us an immense advantage in electrodynamic studies of bound-state systems, like atoms, molecules, and mesoscopic objects: The stationary states of the bound system are calculated from the (many-body) Schrödinger equation approximating the particle-particle interaction by the nonretarded Coulomb interaction, and the transverse electromagnetic field effects, which give rise to retarded dynamic electrodynamic interactions, is treated as a

perturbation. Other formulations, derived from the Coulomb gauge, can also be used with advantage in low-energy studies, as we shall learn in Chaps. 25 and 26.

In recent years, I have advocated that the covariant theory can provide us with a new perspective of near-field electrodynamics, and even be of practical interest for some low-energy near-field calculations [177, 180, 231, 232]. In near-field interactions the dynamic part of the longitudinal electric field always plays an important role, and in a photon description this field involves a combination of longitudinal and scalar photon dynamics. Since the longitudinal electric field relates to the difference between the longitudinal and scalar photon wave functions in the first-quantized theory, it is convenient to introduce, via a unitary transformation, two new types of photons, named gauge and near-field photons [177]. In near-field electrodynamics, just one of the new photon types are needed. In the absence of near-field interactions the near-field photon vanishes, and this is the reason that I have attached the name “near-field” to this new virtual photon type. In Sect. 16.4 the wave mechanics of the gauge and near-field photons is studied.

The photon is a free-field concept, and in near-field electrodynamics photons are never free! The gauge and near-field photons therefore are virtual photons, existing only during particle–particle interaction. In Chap. 18, near-field aspects of photon wave packet emission from micro- and mesoscopic sources are discussed. In a wave mechanical context, the space–time photon release takes place in the rim zone of the source, and we describe the process on the basis of a propagator formalism for what I have called *the photon embryo concept* [180, 229, 232]. To be sure that just one transverse wave packet photon is emitted from the source, the current density distribution must be properly normalized. Using the photon energy wave function formalism, the correct normalization is achieved working in the momentum representation [229].

8.8 Photon Spin and Helicity

The transverse part of the classical electromagnetic field (associated to $\mathbf{E}_T$ and $\mathbf{B}$) possesses angular momentum in general [19, 37–42, 233–235], and this relates to a photon angular momentum [53, 178, 236, 237] in photon wave mechanics [180, 213]. In Chap. 17, the field angular momentum is studied starting from some considerations regarding the bodily rotation of vector fields. It is shown that the generator of infinitesimal vector field rotations is the *sum* of the (dimensionless) orbital ($\hat{\mathbf{L}}$) and spin ($\hat{\mathbf{S}}$) angular momentum operators. To preserve the transverse nature of the photon field only the operator $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ is an observable. Calculations of the quantum mechanical mean values of the orbital and spin angular momenta are carried out in the complex field theory and in the energy wave function formalism. After having studied the so-called projected photon spin operator [238, 239], we finish Chap. 17 with a calculation of the eigenvectors and eigenvalues of the photon helicity operator.

8.9 Superlocalization: One-Particle Position Operators

In a photon emission process, the best spatial confinement of the photon embryo appears in the very first instance of the process, and the spatial localization domain has the extension of the rim zone of the source [180]. The extension of the rim zone is given by that of the transverse current density, $\mathbf{J}_T$. In all processes where the electron configuration of the source is changed during the emission, the spatial photon localization has an R^{-n} extension [$n = 3, 4, \dots$]. For an electric dipole transition $n = 3$. If one could meet the condition

$$\mathbf{J}_T(\mathbf{r}, t) = \mathbf{J}(\mathbf{r}, t), \quad (8.14)$$

the rim zone would be absent, and the photon source region hence confined to a domain comparable to the electronic size of the source. Such a possibility occurs, as we shall realize in Chap. 20, in photon emission from pure spin transitions [176, 179, 180]. In such processes so-called exponential photon source localization appears. As a paradigm for exponential localization stands the birth process of radio-frequency photons emitted from the hyperfine transitions belonging to the hydrogen $1s_{1/2}$ ground state [164, 176, 180]. The $1s$ level has no fine structure, and the $1s$ electron no orbital angular momentum. Only the spin degrees of freedom are involved. In a somewhat indirect manner the photon source localization problem is related to the photon position operator problem [240–246]. In Chap. 21, we study this problem, briefly, starting from a discussion of the position operator problem for massive relativistic particles of zero spin [247–250]. Main emphasis is devoted to a simple analysis of the transverse photon eigenstates in momentum space, and the subsequent introduction of a dyadic photon position operator [251–253].

8.10 Transverse Photon Mass: Eikonal Theory for Photons

At high frequencies the field–matter interaction becomes diamagnetic in nature, and the photon behavior tends to be particle-like. In consequence, a transverse photon propagating through an assumed homogeneous condensed-matter medium attains an effective mass [177]. In Sect. 19.2 we study the transverse photon mass on the basis of photon wave mechanics. The always existing electronic inhomogeneity of a solid medium makes the photon–matter interaction complicated to describe, in general, even at high frequencies. However, if the electron density varies sufficiently slowly in space a photon eikonal description becomes possible [254]. If, in the classical theory of electrodynamics, the finiteness of the wavelength of light can be neglected, the optical laws may be formulated in the language of geometry, and the gradient of the eikonal satisfies the eikonal equation of geometrical optics [43, 44].

The eikonal equation in optics is form-identical to the Hamilton–Jacobi equation for Hamilton’s characteristic function for a single classical particle. After a brief review of the Hamilton–Jacobi formulation [255–258] (Sect. 19.4), we describe the

eikonal theory of charged particles in quantum mechanics (Sect. 19.5). In the non-relativistic regime, the Hamilton–Jacobi equation leads to the de Broglie-Bohm pilot-wave formulation of quantum mechanics [259–267]. The pilot-wave theory for massive particles offers us an interpretation of the foundation of quantum mechanics which appears as an alternative to the Copenhagen interpretation. The philosophy behind the Copenhagen theory is mainly due to Niels Bohr [268–274]. While Bohr agonized over the question *particle or wave*, de Broglie proposed the answer *particle and wave*. Whether or not a pilot-wave theory for a single photon can be formulated appears to be an open question [265].

Chapter 9

Transverse and Longitudinal Electrodynamics

9.1 Solenoidal and Irrotational Vector Fields

9.1.1 Helmholtz Theorem

Let us consider an everywhere differentiable vector field $\mathbf{W}(\mathbf{r})$ which vanishes at infinity. For such a vector field we shall sketch the prove of Helmholtz theorem, viz., that $\mathbf{W}(\mathbf{r})$ may be resolved uniquely into two parts, one of which is irrotational, the other solenoidal [275, 276]. To prove Helmholtz theorem we construct from $\mathbf{W}(\mathbf{r})$ the vector function

$$\mathbf{V}(\mathbf{r}) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \frac{\mathbf{W}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r', \quad (9.1)$$

which is a solution to the vectorial Poisson equation $\nabla^2 \mathbf{V} = -\mathbf{W}$. This equation may also be given in the form $\nabla \times (\nabla \times \mathbf{V}) - \nabla \nabla \cdot \mathbf{V} = \mathbf{W}$, and with the introduction of the scalar and vector potential functions $\phi = -\nabla \cdot \mathbf{V}$, and $\mathbf{\Phi} = \nabla \times \mathbf{V}$ we have

$$\mathbf{W}(\mathbf{r}) = \nabla \phi(\mathbf{r}) + \nabla \times \mathbf{\Phi}(\mathbf{r}). \quad (9.2)$$

Since $\mathbf{V}$ is determined uniquely (by (9.1)), ϕ and $\mathbf{\Phi}$ are determined uniquely. With the notation $\mathbf{W}_T = \nabla \times \mathbf{\Phi}$ and $\mathbf{W}_L = \nabla \phi$, we thus may write

$$\mathbf{W}(\mathbf{r}) = \mathbf{W}_T(\mathbf{r}) + \mathbf{W}_L(\mathbf{r}), \quad (9.3)$$

where

$$\nabla \cdot \mathbf{W}_T(\mathbf{r}) = 0, \quad (9.4)$$

and

$$\nabla \times \mathbf{W}_L(\mathbf{r}) = \mathbf{0}. \quad (9.5)$$

A vector field $\mathbf{W}_T(\mathbf{r})$, which satisfies (9.4) (everywhere within its domain of definition – here the entire space) is called solenoidal (or divergence-free, or, as is common in (quantum) electrodynamics, transverse (therefore, subscript T)). The curl of $\mathbf{W}_T$ is given by $\nabla \times \mathbf{W}_T = \nabla \times (\nabla \times \mathbf{\Phi})$. The vector field $\mathbf{W}_L(\mathbf{r})$, which

satisfies (9.5) everywhere, is called irrotational (or rotational-free, or longitudinal (L)). The divergence of $\mathbf{W}_L$ is given by $\nabla \cdot \mathbf{W}_L = \nabla^2 \phi$. The result in (9.3)–(9.5) is Helmholtz theorem. It appears from the analysis above that

$$\mathbf{W}_T(\mathbf{r}) = \nabla \times \left(\nabla \times \int_{-\infty}^{\infty} \frac{\mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} d^3 r' \right), \quad (9.6)$$

and

$$\mathbf{W}_L(\mathbf{r}) = -\nabla \nabla \cdot \int_{-\infty}^{\infty} \frac{\mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} d^3 r'. \quad (9.7)$$

The transverse and longitudinal parts of $\mathbf{W}(\mathbf{r})$ hence are related in a spatially non-local manner to $\mathbf{W}(\mathbf{r})$. If we choose to base our theoretical studies of near-field electrodynamics phenomena on a L–T division of the various vector fields which occur in the Maxwell–Lorentz equations, it is of central importance for a correct understanding of the physics to fully appreciate this spatial nonlocality. Calculations based on a L–T division, a covariant formulation, and other equivalent theoretical schemes must of course lead to identical predictions for observable quantities. Approximations are in general made in theoretical calculations, but it is not always easy to ensure that these are done equivalently in the various schemes! New insight is often obtained by looking at the same problem from various perspectives.

If one in (9.6) and (9.7), (1) interchanges the ∇ – and integral operations (and this can be done without danger), (2) uses that $\nabla |\mathbf{r} - \mathbf{r}'|^{-1} = -\nabla' |\mathbf{r} - \mathbf{r}'|^{-1}$, (3) carries out certain partial integrations (the surface terms at infinity vanish), and finally (4) makes use of (9.3), one obtains the vector identity

$$\mathbf{W}(\mathbf{r}) = \nabla \times \int_{-\infty}^{\infty} \frac{\nabla' \times \mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} d^3 r' - \nabla \int_{-\infty}^{\infty} \frac{\nabla' \cdot \mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} d^3 r'. \quad (9.8)$$

As a corollary to the Helmholtz theorem, (9.8) tells us that the vector field $\mathbf{W}(\mathbf{r})$ is uniquely specified by giving its divergence and its curl everywhere in space. The corollary can be generalized to: A vector field is uniquely specified by giving its divergence and its curl within a simply connected region and its normal component over the boundary.

9.1.2 Decomposition in Reciprocal Space

The prescription in (4.15) immediately shows that (9.4) and (9.5) take a particularly simple form in reciprocal ($\mathbf{q}$) space. Thus,

$$\mathbf{q} \cdot \mathbf{W}_T(\mathbf{q}) = 0, \quad (9.9)$$

$$\mathbf{q} \times \mathbf{W}_L(\mathbf{q}) = \mathbf{0}. \quad (9.10)$$

The names transverse (T) and longitudinal (L) thus have a clear geometrical significance in reciprocal space: $\mathbf{W}_T(\mathbf{q})$ is perpendicular to $\mathbf{q}$ (for all $\mathbf{q}$), and $\mathbf{W}_L(\mathbf{q})$ is parallel to $\mathbf{q}$. The complicated nonlocal relations between $\mathbf{W}_T(\mathbf{r})$ [$\mathbf{W}_L(\mathbf{r})$] and $\mathbf{W}(\mathbf{r})$ given in (9.6) and (9.7) are replaced by simple algebraic relations, namely

$$\mathbf{W}_T(\mathbf{q}) = (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{W}(\mathbf{q}), \quad (9.11)$$

$$\mathbf{W}_L(\mathbf{q}) = \hat{\mathbf{q}}\hat{\mathbf{q}} \cdot \mathbf{W}(\mathbf{q}), \quad (9.12)$$

where $\hat{\mathbf{q}} = \mathbf{q}/q$. The relations in (9.11) and (9.12) are readily obtained from (9.9) and (9.10), remembering that $\mathbf{W}(\mathbf{q}) = \mathbf{W}_T(\mathbf{q}) + \mathbf{W}_L(\mathbf{q})$. In reciprocal space the relationships which exist between a vector field and its transverse and longitudinal parts are local: $\mathbf{W}_T$ and $\mathbf{W}_L$ at a given $\mathbf{q}$ -point are related to $\mathbf{W}$ at the same point, only. It is important to emphasize that a vector *field* is transverse (longitudinal) only if (9.9) [(9.10)] holds for all $\mathbf{q}$. The dyadic quantities

$$\delta_T(\mathbf{q}) = \mathbf{U} - q^{-2}\mathbf{q}\mathbf{q}, \quad (9.13)$$

and

$$\delta_L(\mathbf{q}) = q^{-2}\mathbf{q}\mathbf{q}, \quad (9.14)$$

which are projectors enabling one to obtain $\mathbf{W}_T(\mathbf{q})$ and $\mathbf{W}_L(\mathbf{q})$ from $\mathbf{W}(\mathbf{q})$ are important in near-field electrodynamics, and they are called the transverse and longitudinal delta function, respectively, for a reason to be discussed below.

9.1.3 Transverse and Longitudinal Delta-Function Dyadics

In certain contexts, it is useful to seek to interchange the integral and differential [$\nabla \times (\nabla \times)$, $-\nabla \nabla \cdot$] operations in (9.6) and (9.7). One cannot just interchange these operations, because the double nabla operations on $\mathbf{W}(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'|$ lead to integrands with a singularity of the type $|\mathbf{r} - \mathbf{r}'|^{-3}$. Such a singularity makes the integrals only conditionally convergent, and this is incompatible with the fact that the original equations (9.6) and (9.7) determine $\mathbf{W}_T(\mathbf{r})$ and $\mathbf{W}_L(\mathbf{r})$ unconditionally. A careful analysis [18] shows that one may take

$$\mathbf{W}_T(\mathbf{r}) = P \int_{-\infty}^{\infty} \nabla \times \left[\nabla \times \left(\frac{\mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} \right) \right] d^3r' + \frac{2}{3}\mathbf{W}(\mathbf{r}), \quad (9.15)$$

and

$$\mathbf{W}_L(\mathbf{r}) = -P \int_{-\infty}^{\infty} \nabla \nabla \cdot \left(\frac{\mathbf{W}(\mathbf{r}')}{4\pi |\mathbf{r} - \mathbf{r}'|} \right) d^3r' + \frac{1}{3}\mathbf{W}(\mathbf{r}), \quad (9.16)$$

where P means that the principal value of the subsequent conditionally convergent integral is to be taken. *Here*, the P -integration is carried out by first removing a small *spherical* volume of radius ϵ from the integration domain. The sphere is

centered on the point $\mathbf{r}$, and after the integration has been done, one takes the limit $\epsilon \rightarrow 0$. The P -integrals represent the spatially nonlocal contributions to $\mathbf{W}_T(\mathbf{r})$ and $\mathbf{W}_L(\mathbf{r})$, and the terms $2\mathbf{W}(\mathbf{r})/3$ and $\mathbf{W}(\mathbf{r})/3$ give the local contributions to these vector fields. It is important to emphasize that it is possible to make other choices for the form of the infinitesimal exclusion volume than the spherical. In such cases, both the nonlocal contributions from the P -integration and the local contribution would be different from the ones in (9.15) and (9.16). The sum of the two contributions will be independent of the form of the exclusion volume. Due to the fact that the speed of light in vacuum is isotropic, it is often natural to choose a spherical exclusion volume in theoretical studies of the near-field electrodynamics of microscopic and mesoscopic objects, when the calculations are based on the T-L split of the various vector fields. By addition of (9.15) and (9.16) the integral terms cancel and we obtain (9.3).

Once the differential and integral operations have been interchanged the relations of $\mathbf{W}_T$ and $\mathbf{W}_L$ to $\mathbf{W}$ can be written in the compact forms

$$\mathbf{W}_T(\mathbf{r}) = \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \mathbf{W}(\mathbf{r}') d^3 r', \quad (9.17)$$

and

$$\mathbf{W}_L(\mathbf{r}) = \int_{-\infty}^{\infty} \delta_L(\mathbf{r} - \mathbf{r}') \cdot \mathbf{W}(\mathbf{r}') d^3 r'. \quad (9.18)$$

The dyadic nonlocal functions $\delta_T(\mathbf{r} - \mathbf{r}')$ and $\delta_L(\mathbf{r} - \mathbf{r}')$ are the so-called transverse and longitudinal delta functions. They are named so because they project out from the vector field $\mathbf{W}(\mathbf{r}')$ its transverse and longitudinal components at a given point $(\mathbf{r})$. By carrying out the differential operations in (9.15) and (9.16) one obtains the following dyadic expressions for the delta functions:

$$\delta_T(\mathbf{R}) = -\frac{U - 3\hat{\mathbf{R}}\hat{\mathbf{R}}}{4\pi R^3} + \frac{2}{3}\delta(\mathbf{R})U, \quad (9.19)$$

and

$$\delta_L(\mathbf{R}) = \frac{U - 3\hat{\mathbf{R}}\hat{\mathbf{R}}}{4\pi R^3} + \frac{1}{3}\delta(\mathbf{R})U. \quad (9.20)$$

It must be remembered that the formulas in (9.19) and (9.20) relate to spherical contraction. The importance of these transverse and longitudinal delta functions for near-field electrodynamics stems from the fact that they couple $\mathbf{W}_T$ and $\mathbf{W}_L$ to $\mathbf{W}$ over near-field zone (R^{-3}) distances. Both dyadic delta functions are singular at $\mathbf{R} = \mathbf{0}$, and by addition it appears that the sum

$$\delta_T(\mathbf{R}) + \delta_L(\mathbf{R}) = \delta(\mathbf{R})U \quad (9.21)$$

is just the usual Dirac delta function multiplied by the unit tensor.

9.2 Transverse and Longitudinal Parts of the Maxwell–Lorentz Equations

9.2.1 Field Equations in Direct Space

It appears from the Maxwell–Lorentz equation in (2.4) that the magnetic field is a purely transverse vector field, i.e.,

$$\mathbf{B}(\mathbf{r}, t) = \mathbf{B}_T(\mathbf{r}, t). \quad (9.22)$$

It is evident from the Maxwell–Lorentz equations in (2.1) and (2.2) that the electric field, in general, has both T- and L-parts. Thus,

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_T(\mathbf{r}, t) + \mathbf{E}_L(\mathbf{r}, t). \quad (9.23)$$

It must be stressed here that although the electric field outside matter, where $\rho(\mathbf{r}, t) = 0$, satisfies the condition $\nabla \cdot \mathbf{E}(\mathbf{r}, t) = 0$ everywhere, $\mathbf{E}$ in general is *not* a transverse vector field because its domain of definition (all space) also includes matter-field regions where $\nabla \cdot \mathbf{E} = \rho$. Solely in the exceptional cases where only pure spin transitions are involved in the electrodynamics will the electric field be a transverse vector field; see Chap. 20. Even in the microscopic classical theory, where all charged particles are point entities distributed discretely in space will the electric field not be a transverse vector field. For a single point particle with charge Q and located at $\mathbf{r} = \mathbf{r}_Q(t)$, one has $\nabla \cdot \mathbf{E} = 0$ everywhere in space except at one point (the instantaneous location of the particle), and $\mathbf{E}$ is therefore not a transverse vector field! The considerations above are exemplified in Fig. 9.1, which refers also to Sect. 9.2.2. Perhaps, the aforementioned conclusion is even more evident in reciprocal space where $i\epsilon_0 \mathbf{q} \cdot \mathbf{E}_T(\mathbf{q}, t) = Q \exp(-i\mathbf{q} \cdot \mathbf{r}_Q(t))$, as the reader may show. In $\mathbf{q}$ -space $\mathbf{q} \cdot \mathbf{E}_T(\mathbf{q}, t)$, hence, is nonvanishing everywhere. The current density also has both T- and L-parts in general, i.e.,

$$\mathbf{J}(\mathbf{r}, t) = \mathbf{J}_T(\mathbf{r}, t) + \mathbf{J}_L(\mathbf{r}, t). \quad (9.24)$$

There exists an important exception, however: In a pure spin transition, the associated transition current density flow is incompressible, and this means that $\mathbf{J} = \mathbf{J}_T$, everywhere. The spin case is of significant importance for a fundamental discussion of where the limits are (if they exist) for the spatial super resolution in near-field optics, as we shall understand later on, in Chap. 20.

By means of the decompositions in (9.22)–(9.24), the Maxwell–Lorentz equations in (2.1)–(2.4) can be divided into a set

$$\nabla \times \mathbf{E}_T(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t), \quad (9.25)$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \mu_0 \mathbf{J}_T(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{r}, t), \quad (9.26)$$

Fig. 9.1 Schematic illustration of rim zones (in the *light grey* tone) of some charge density distributions (in *dark grey* tone). *Top figure*: Point-particle. The rim zone has an R^{-3} -profile. *Middle figure*: Mesoscopic object. The rim zone is given by the last term in (9.32). *Bottom figure*: Plane surface of a translationally invariant medium filling a halfspace. The rim zone has the form of an exponentially decaying (evanescent) tail



describing the transverse electrodynamics [$\nabla \cdot \mathbf{E}_T(\mathbf{r}, t) = \nabla \cdot \mathbf{B}(\mathbf{r}, t) = \nabla \cdot \mathbf{J}_T(\mathbf{r}, t) = 0$], and a set

$$\mathbf{J}_L(\mathbf{r}, t) + \epsilon_0 \frac{\partial}{\partial t} \mathbf{E}_L(\mathbf{r}, t) = \mathbf{0}, \quad (9.27)$$

$$\nabla \cdot \mathbf{E}_L(\mathbf{r}, t) = \frac{1}{\epsilon_0} \rho(\mathbf{r}, t), \quad (9.28)$$

governing the longitudinal electrodynamics [$\nabla \times \mathbf{E}_L(\mathbf{r}, t) = \nabla \times \mathbf{J}_L(\mathbf{r}, t) = \mathbf{0}$]. The information in the two Maxwell–Lorentz equations (2.1) and (2.4) is contained in (9.22) and (9.25), and the field equations in (2.2) and (9.28) are equivalent. The Helmholtz decomposition of (2.3) leads to (9.26) and (9.27) (use also $\mu_0 c_0^2 = \epsilon_0^{-1}$). The equation of charge continuity is contained in (9.27) and (9.28): From (9.27) one gets $\nabla \cdot \mathbf{J}_L + \epsilon_0 \partial \nabla \cdot \mathbf{E}_L / \partial t = 0$, and by eliminating $\nabla \cdot \mathbf{E}_L$ with the help of (9.28) one obtains $\nabla \cdot \mathbf{J} + \partial \rho / \partial t = 0$, i.e., (2.108). The longitudinal part of the electric field is related in a spatially and timely nonlocal manner to the current density, as may be seen by integrating (9.27) between a reference time t_0 and t , and by using afterwards (9.18) to replace $\mathbf{J}_L$ by $\mathbf{J}$. Thus,

$$\mathbf{E}_L(\mathbf{r}, t) = \mathbf{E}_L(\mathbf{r}, t_0) - \frac{1}{\epsilon_0} \int_{t_0}^t \int_{-\infty}^{\infty} \delta_L(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}', t') d^3 r' dt'. \quad (9.29)$$

The longitudinal electrodynamics governed by (9.27) and (9.28) does not involve the speed of light in vacuum, and the longitudinal electric field is *not* related to

the current density via a wave equation albeit the relation between $\mathbf{E}_L(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}', t')$ is nonlocal in space and time. The transverse dynamics on the other hand does give rise to inhomogeneous wave equations for the transverse electric field and the magnetic field, viz.,

$$\square \mathbf{E}_T(\mathbf{r}, t) = \mu_0 \frac{\partial}{\partial t} \mathbf{J}_T(\mathbf{r}, t), \quad (9.30)$$

and

$$\square \mathbf{B}(\mathbf{r}, t) = -\mu_0 \nabla \times \mathbf{J}(\mathbf{r}, t), \quad (9.31)$$

as the reader may verify by combination of (9.25) and (9.26) in the usual manner. In the perspective of near-field electrodynamics, there is an important difference between the extensions of the source regions for the magnetic field and the transverse electric field: Roughly speaking the source region of $\mathbf{B}$ coincides with the region in space where the charge current density itself, $\mathbf{J}(\mathbf{r}, t)$, is nonvanishing, whereas the source region of $\mathbf{E}_T$ is the part of space where the transverse current density, $\mathbf{J}_T(\mathbf{r}, t)$, is nonvanishing, and for a microscopic or mesoscopic source $\mathbf{J}_T$ will in general be nonzero in the entire near-field region of $\mathbf{J}$, cf. (9.17) and (9.19).

9.2.2 Rim Zone of Matter

In spherical contraction, the spatially nonlocal relation between $\mathbf{J}(\mathbf{r}, t)$ and $\mathbf{J}_L(\mathbf{r}, t)$ is given by

$$\mathbf{J}_L(\mathbf{r}, t) = \frac{1}{3} \mathbf{J}(\mathbf{r}, t) + \frac{1}{4\pi} P \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-3} (U - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) \cdot \mathbf{J}(\mathbf{r}', t) d^3 r', \quad (9.32)$$

and it appears from this connection, and (9.27) and (9.28) that the longitudinal electrodynamics plays a central role inside matter and in a narrow zone outside matter. The current density in (9.32) may be that of a microscopic, mesoscopic or macroscopic source. The longitudinal vector fields $\mathbf{E}_L(\mathbf{r}, t)$ and $\mathbf{J}_L(\mathbf{r}, t)$ are related in a spatially *local* manner, see (9.27), and outside matter, where $\rho(\mathbf{r}, t) = 0$, the longitudinal electric field is divergence-free, i.e.,

$$\nabla \cdot \mathbf{E}_L(\mathbf{r}, t) = 0. \quad (9.33)$$

I have called the region in space where (9.33) is satisfied, and $\mathbf{E}_L(\mathbf{r}, t) \neq 0$, the rim zone of matter [177]. Per definition $\nabla \times \mathbf{E}_L(\mathbf{r}, t) = \mathbf{0}$ everywhere in space, and thus also in the rim zone. A summary of the T–L vector fields distribution in space is shown in Table 9.1.

Table 9.1 Survey of the transverse and longitudinal parts of the electric field and the current density in the various regions of space: (1) The $\mathbf{J}$ -domain, where the microscopic charge density is nonvanishing, (2) the rim (or near-field) zone, and (3) the rest of space, where only transverse electromagnetic fields can exist

$\mathbf{J}$ -domain	Rim zone	Rest of space
Photon source domain		
$\mathbf{J}_T + \mathbf{J}_L = \mathbf{J} \neq \mathbf{0}$	$\mathbf{J}_T = -\mathbf{J}_L = \mathbf{0}$	$\mathbf{J}_T = \mathbf{J}_L = \mathbf{0}$
$\mathbf{E}_L \neq \mathbf{0}$		$\mathbf{E}_L = \mathbf{0}$
$\nabla \cdot \mathbf{E}_L = \rho$	$\nabla \cdot \mathbf{E}_L = 0$	
$\mathbf{E}_T \neq \mathbf{0}$		
$\nabla \times \mathbf{E}_T = -\partial \mathbf{B} / \partial t$		

9.2.3 Field Equations in Reciprocal Space

The translation in (4.15) immediately allows one to write down the L- and T-sets of the Maxwell–Lorentz equations in reciprocal space. Hence, the two transverse field equations in (9.25) and (9.26) take the form

$$i\mathbf{q} \times \mathbf{E}_T(\mathbf{q}; t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{q}; t), \quad (9.34)$$

$$i\mathbf{q} \times \mathbf{B}(\mathbf{q}; t) = \mu_0 \mathbf{J}_T(\mathbf{q}; t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{q}; t), \quad (9.35)$$

and the longitudinal field equations in (9.27) and (9.28) become

$$\mathbf{J}_L(\mathbf{q}; t) + \epsilon_0 \frac{\partial}{\partial t} \mathbf{E}_L(\mathbf{q}; t) = \mathbf{0}, \quad (9.36)$$

$$i\mathbf{q} \cdot \mathbf{E}_L(\mathbf{q}; t) = \frac{1}{\epsilon_0} \rho(\mathbf{q}; t). \quad (9.37)$$

9.2.4 Potential Description

The vector potential plays a central role in the quantum theory of near-field electrodynamics as we shall realize later on in this book. If one splits the vector potential into its transverse and longitudinal parts, i.e.,

$$\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_T(\mathbf{r}, t) + \mathbf{A}_L(\mathbf{r}, t), \quad (9.38)$$

it appears from (2.5) that the magnetic field

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}_T(\mathbf{r}, t), \quad (9.39)$$

is determined by the transverse part of $\mathbf{A}(\mathbf{r}, t)$. This fact of course originates in our freedom of making an arbitrary choice for the divergence of $\mathbf{A}(\mathbf{r}, t)$, $\nabla \cdot \mathbf{A}(\mathbf{r}, t) = \nabla \cdot \mathbf{A}_L(\mathbf{r}, t)$. The transverse part of the electric field can be obtained solely from the transverse part of the vector potential, whereas the longitudinal part of the electric field relates not only to the longitudinal part of the vector potential but also to the scalar potential. Thus, we obtain from (2.7) the following relations:

$$\mathbf{E}_T(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{A}_T(\mathbf{r}, t), \quad (9.40)$$

$$\mathbf{E}_L(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{A}_L(\mathbf{r}, t) - \nabla \phi(\mathbf{r}, t). \quad (9.41)$$

It appears from (2.11) that the transverse part of the vector potential is gauge invariant, i.e.,

$$\mathbf{A}_T(\mathbf{r}, t) \Rightarrow \mathbf{A}'_T(\mathbf{r}, t) = \mathbf{A}_T(\mathbf{r}, t). \quad (9.42)$$

This agrees with the fact that the gauge invariant vector fields $\mathbf{E}_T(\mathbf{r}, t)$ and $\mathbf{B}_T(\mathbf{r}, t)$ depend on $\mathbf{A}_T(\mathbf{r}, t)$, only. The longitudinal part of the vector potential transforms as follows:

$$\mathbf{A}_L(\mathbf{r}, t) \Rightarrow \mathbf{A}'_L(\mathbf{r}, t) = \mathbf{A}_L(\mathbf{r}, t) + \nabla \chi(\mathbf{r}, t). \quad (9.43)$$

The gauge transforms in (2.12) and (9.43) ensure the gauge invariance of the longitudinal electric field in (9.41). By division of the wave equation for the vector potential (2.9) into its T- and L-parts one obtains

$$\square \mathbf{A}_T(\mathbf{r}, t) = -\mu_0 \mathbf{J}_T(\mathbf{r}, t), \quad (9.44)$$

and

$$\square \mathbf{A}_L(\mathbf{r}, t) - \nabla \left(\nabla \cdot \mathbf{A}_L(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \phi(\mathbf{r}, t) \right) = -\mu_0 \mathbf{J}_L(\mathbf{r}, t). \quad (9.45)$$

Differentiation of (9.44) with respect to time, and use afterwards of (9.40) lead us back to (9.30). In order to determine the framework for the longitudinal electrodynamics from a potential description, (9.45) must be supplemented by the equation

$$\nabla^2 \phi(\mathbf{r}, t) + \frac{\partial}{\partial t} \nabla \cdot \mathbf{A}_L(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \rho(\mathbf{r}, t), \quad (9.46)$$

cf. (2.8). In the Lorenz gauge, where

$$\nabla \cdot \mathbf{A}_L(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \phi(\mathbf{r}, t) = 0, \quad (9.47)$$

the longitudinal part of the vector potential satisfies the wave equation

$$\square \mathbf{A}_L(\mathbf{r}, t) = -\mu_0 \mathbf{J}_L(\mathbf{r}, t), \quad (9.48)$$

and the addition of (9.44) and (9.45) of course gives (2.14). In the Coulomb gauge, where the choice

$$\nabla \cdot \mathbf{A}(\mathbf{r}, t) = \nabla \cdot \mathbf{A}_L(\mathbf{r}, t) = 0 \quad (9.49)$$

is made, in every space point (inside and outside matter-filled regions), the scalar potential satisfies the (quasi-static) Poisson equation

$$\nabla^2 \phi(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \rho(\mathbf{r}, t). \quad (9.50)$$

The solution to this equation is given by the nonretarded ($c_0 \rightarrow \infty$) version of (2.20). Since $\nabla \times \mathbf{A}_L(\mathbf{r}, t) = \mathbf{0}$ per definition, it follows from the vector identity in (9.8) with $\mathbf{W} = \mathbf{A}_L$ that

$$\mathbf{A}_L(\mathbf{r}, t) = \mathbf{0} \quad (9.51)$$

in the Coulomb gauge. In consequence, $\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_T(\mathbf{r}, t)$ in this gauge.

9.3 Role of the Longitudinal Electric Field

9.3.1 Instantaneous Coulomb Field

If one uses the vector identity in (9.8) on the longitudinal part of the electric field, i.e., $\mathbf{W} = \mathbf{E}_L(\mathbf{r}, t)$, one immediately gets

$$\mathbf{E}_L(\mathbf{r}, t) = -\nabla \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}', t)}{4\pi\epsilon_0 |\mathbf{r} - \mathbf{r}'|} d^3r', \quad (9.52)$$

and then

$$\mathbf{E}_L(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \rho(\mathbf{r}', t) d^3r'. \quad (9.53)$$

For an assembly of point-particles, where $\rho(\mathbf{r}', t)$ is given by (2.28), the longitudinal electric field becomes

$$\mathbf{E}_L(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \sum_{\alpha} \frac{q_{\alpha}(\mathbf{r} - \mathbf{r}_{\alpha}(t))}{|\mathbf{r} - \mathbf{r}_{\alpha}(t)|^3}. \quad (9.54)$$

Hence, it is realized that the longitudinal electric field at time t is the “Coulomb field” associated with ρ , and calculated as if ρ were static and assumed to have its value taken at t . The longitudinal electric field is therefore called the instantaneous

Coulomb field of the charge distribution. Relativistically, $\mathbf{E}_L(\mathbf{r}, t)$ can be obtained from the sum of the velocity fields of the various charges, taking these velocity fields in the limit $c_0 \rightarrow \infty$, cf. (2.61). It is not surprising that the longitudinal electric field appears in this limit because an instantaneous Coulomb field from a charge distribution in motion can only be obtained if the speed of light can be considered as infinitely high. The electric velocity field of the point charge distribution also has a transverse part, and the sum of the transverse and longitudinal parts is retarded, cf. (2.61). In the Coulomb gauge, where $\mathbf{A}_L(\mathbf{r}, t) = \mathbf{0}$ (see (9.51)), the longitudinal field is given by $\mathbf{E}_L(\mathbf{r}, t) = -\nabla\phi(\mathbf{r}, t)$ (see (9.41)), and a comparison to (9.52) immediately leads to the instantaneous Coulomb (scalar) potential of the charge distribution:

$$\phi(\mathbf{r}, t) = \frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3r'. \quad (9.55)$$

9.3.2 Coulomb Interaction and Self-Energy

In the following analysis, it is profitable to make use of the Parseval–Plancherel identity

$$\int_{-\infty}^{\infty} V^*(\mathbf{r})W(\mathbf{r})d^3r = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} V^*(\mathbf{q})W(\mathbf{q})d^3q, \quad (9.56)$$

where $V(\mathbf{q})$ and $W(\mathbf{q})$ are the spatial Fourier integral transforms of the functions $V(\mathbf{r})$ and $W(\mathbf{r})$ (cf. the spatial parts of the transformations in (4.13) and (4.14)). By insertion of the Fourier integral expressions for $V^*(\mathbf{r})$ and $W(\mathbf{r})$ on the left side of (9.56) it is not difficult, with the help of the plane-wave expansion of the Dirac delta function (4.23), to prove the correctness of (9.56). The Parseval–Plancherel identity allows one to write the electric field part of the field energy in (2.75) in the form

$$\frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) d^3r = \left(\frac{1}{2\pi}\right)^3 \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}^*(\mathbf{q}; t) \cdot \mathbf{E}(\mathbf{q}; t) d^3q, \quad (9.57)$$

and if one subsequently splits the electric field into its T- and L-parts, $\mathbf{E}(\mathbf{q}; t) = \mathbf{E}_T(\mathbf{q}; t) + \mathbf{E}_L(\mathbf{q}; t)$, and uses the orthogonality of these parts in reciprocal space, i.e., $\mathbf{E}_T(\mathbf{q}; t) \cdot \mathbf{E}_L(\mathbf{q}; t) = 0$ (and thus also $\mathbf{E}_T^* \cdot \mathbf{E}_L = \mathbf{E}_T \cdot \mathbf{E}_L^* = 0$ in $\mathbf{q}$ -space) one yields

$$\begin{aligned} \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t) d^3r &= \left(\frac{1}{2\pi}\right)^3 \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}_L^*(\mathbf{q}; t) \cdot \mathbf{E}_L(\mathbf{q}; t) d^3q \\ &\quad + \left(\frac{1}{2\pi}\right)^3 \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}_T^*(\mathbf{q}; t) \cdot \mathbf{E}_T(\mathbf{q}; t) d^3q. \end{aligned} \quad (9.58)$$

The first term on the right side of (9.58) is the contribution of the longitudinal electric field to the field energy in (2.75). We name this contribution H_{long} . Hence,

$$\begin{aligned} H_{\text{long}} &= \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}_L(\mathbf{r}, t) \cdot \mathbf{E}_L(\mathbf{r}, t) d^3r \\ &= \left(\frac{1}{2\pi}\right)^3 \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \mathbf{E}_L^*(\mathbf{q}; t) \cdot \mathbf{E}_L(\mathbf{q}; t) d^3q \\ &= \left(\frac{1}{2\pi}\right)^3 \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \hat{\mathbf{q}} \cdot \mathbf{E}_L^*(\mathbf{q}; t) \hat{\mathbf{q}} \cdot \mathbf{E}_L(\mathbf{q}; t) d^3q. \end{aligned} \quad (9.59)$$

The last equality in (9.59) follows readily via the identity $\mathbf{E}_L(\mathbf{q}; t) = \hat{\mathbf{q}} \hat{\mathbf{q}} \cdot \mathbf{E}_L(\mathbf{q}; t)$, and its complex conjugate. The Maxwell–Lorentz equation in (9.37) in turn gives

$$H_{\text{long}} = \left(\frac{1}{2\pi}\right)^3 \frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \rho^*(\mathbf{q}; t) \rho(\mathbf{q}; t) \frac{d^3q}{q^2}. \quad (9.60)$$

By means of the folding theorem

$$[f * g](\mathbf{r}) \equiv \int_{-\infty}^{\infty} f(\mathbf{r} - \mathbf{r}') g(\mathbf{r}') d^3r' = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} f(\mathbf{q}) g(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3q, \quad (9.61)$$

and the Fourier relation

$$\frac{1}{4\pi R} = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot \mathbf{R}} \frac{d^3q}{q^2} \quad (9.62)$$

one obtains

$$\left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} \rho(\mathbf{q}; t) \frac{d^3q}{q^2} = \frac{1}{4\pi} \int_{-\infty}^{\infty} \rho(\mathbf{r}', t) \frac{d^3r'}{|\mathbf{r} - \mathbf{r}'|}. \quad (9.63)$$

This result and the Parseval–Plancherel identity in (9.56) together show that the expression for H_{long} given in (9.60) can be transformed to

$$H_{\text{long}} = \frac{1}{8\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho(\mathbf{r}, t) \rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3r' d^3r. \quad (9.64)$$

Equation (9.64) tells us that H_{long} is nothing more than the instantaneous Coulomb energy, V_{Coul} , of the charge distribution $\rho(\mathbf{r}, t)$. For a system of point particles with a charge density given by (2.28) one has

$$\rho(\mathbf{q}; t) = \sum_{\alpha} q_{\alpha} e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}(t)}, \quad (9.65)$$

and if one inserts this expression for $\rho(\mathbf{q}; t)$ into (9.60) one gets

$$H_{\text{long}} = V_{\text{Coul}} = \sum_{\alpha} \epsilon_{\text{self}}^{\alpha} + \left(\frac{1}{2\pi} \right)^3 \frac{1}{2\epsilon_0} \sum_{\alpha \neq \beta} q_{\alpha} q_{\beta} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot (\mathbf{r}_{\alpha}(t) - \mathbf{r}_{\beta}(t))} \frac{d^3 q}{q^2}, \quad (9.66)$$

where

$$\epsilon_{\text{self}}^{\alpha} = \left(\frac{1}{2\pi} \right)^3 \frac{q_{\alpha}^2}{2\epsilon_0} \int_{-\infty}^{\infty} \frac{d^3 q}{q^2} \quad (9.67)$$

is the Coulomb self-energy of particle α . For a point particle $\epsilon_{\text{self}}^{\alpha}$ is infinite. The integral in (9.66) is calculated via (9.62), and hence one obtains

$$H_{\text{long}} = V_{\text{Coul}} = \sum_{\alpha} \epsilon_{\text{self}}^{\alpha} + \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha}(t) - \mathbf{r}_{\beta}(t)|}. \quad (9.68)$$

The last term in (9.68) represents the instantaneous Coulomb energy between pairs of particles (α, β) . It appears from (2.72), (2.75), (2.76), (9.58) and (9.66) (first part) that the total energy of the particle-field system is given by

$$H = c_0^2 \sum_{\alpha} m_{\alpha} \gamma_{\alpha} + V_{\text{Coul}} + H_{\text{trans}}, \quad (9.69)$$

where

$$H_{\text{trans}} = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} (\mathbf{E}_{\text{T}}^2(\mathbf{r}, t) + c_0^2 \mathbf{B}^2(\mathbf{r}, t)) d^3 r \quad (9.70)$$

is the energy of the transverse part of the electromagnetic field, a part determined by $\mathbf{E}_{\text{T}}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$. In the nonrelativistic limit, where $H - c_0^2 \sum_{\alpha} m_{\alpha}$ is the relevant total energy, one has

$$H - c_0^2 \sum_{\alpha} m_{\alpha} = \sum_{\alpha} \frac{1}{2} m_{\alpha} v_{\alpha}^2 + V_{\text{Coul}} + H_{\text{trans}}. \quad (9.71)$$

Since the rest energy $c_0^2 \sum_{\alpha} m_{\alpha}$ plays no part in nonrelativistic electrodynamics, we shall later on in this book in sections where we deal with nonrelativistic effects denote the right side of (9.71) just by H .

9.3.3 Particle Momentum Associated with the Longitudinal Electric Field

If the division in (9.23) is inserted into (2.89), the longitudinal electric field gives a contribution

$$\mathbf{P}_{\text{long}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{E}_{\text{L}}(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t) d^3 r = \left(\frac{1}{2\pi} \right)^3 \epsilon_0 \int_{-\infty}^{\infty} \mathbf{E}_{\text{L}}^*(\mathbf{q}; t) \times \mathbf{B}(\mathbf{q}; t) d^3 q \quad (9.72)$$

to the field momentum. The last equality in (9.72) follows readily from the Parseval–Plancherel identity (9.56). Since the longitudinal electric field can be identified as the instantaneous Coulomb field (9.54), or equivalently, the electric velocity field of the particles in the nonretarded ($c_0 \rightarrow \infty$) limit ((2.61) for $\boldsymbol{\beta} \rightarrow \mathbf{0}$), one may guess that $\mathbf{P}_{\text{long}}$ may be expressed solely as a function of the particle position coordinates. That this guess is correct can be shown by insertion of the relations

$$\mathbf{E}_L(\mathbf{q}; t) = \frac{\mathbf{q}}{i\epsilon_0 q^2} \rho(\mathbf{q}; t), \quad (9.73)$$

and $\mathbf{B}(\mathbf{q}; t) = i\mathbf{q} \times \mathbf{A}(\mathbf{q}; t)$ into (9.72) ((9.73) follows from (9.37) by multiplying this equation by $\mathbf{q}/(iq^2)$). Hence, we obtain

$$\mathbf{P}_{\text{long}} = -\left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} \rho^*(\mathbf{q}; t) q^{-2} \mathbf{q} \times (\mathbf{q} \times \mathbf{A}(\mathbf{q}; t)) d^3 q, \quad (9.74)$$

and hereafter

$$\mathbf{P}_{\text{long}} = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} \rho^*(\mathbf{q}; t) (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{A}(\mathbf{q}; t) d^3 q. \quad (9.75)$$

The algebraic relation in (9.11) implies that the expression for $\mathbf{P}_{\text{long}}$ can be written in the form

$$\mathbf{P}_{\text{long}} = \left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} \rho^*(\mathbf{q}; t) \mathbf{A}_T(\mathbf{q}; t) d^3 q, \quad (9.76)$$

where $\mathbf{A}_T(\mathbf{q}; t)$ is the transverse part of the vector potential in the $\mathbf{q}$ -domain. The Parseval–Plancherel identity (9.56) implies that the longitudinal part of the field momentum also may be expressed as

$$\mathbf{P}_{\text{long}} = \int_{-\infty}^{\infty} \rho(\mathbf{r}; t) \mathbf{A}_T(\mathbf{r}, t) d^3 r. \quad (9.77)$$

For an assembly of point particles, where $\rho(\mathbf{r}, t)$ is given by (2.28), one finally gets

$$\mathbf{P}_{\text{long}} = \sum_{\alpha} q_{\alpha} \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t). \quad (9.78)$$

The suspicion that $\mathbf{P}_{\text{long}}$ might be expressed solely as a function of the particle position coordinates thus has turned out to be correct. It is remarkable that the longitudinal field momentum only depends on (the transverse part of) the vector potentials at the various particle positions. Since $\mathbf{P}_{\text{long}}$ is gauge invariant it is not surprising that only the gauge invariant transverse part of the vector potential enters (9.78). The total momentum of the global field–particle system (2.87) now can be written as follows:

$$\mathbf{P} = \sum_{\alpha} (\boldsymbol{\pi}_{\alpha} + q_{\alpha} \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t)) + \mathbf{P}_{\text{trans}}, \quad (9.79)$$

where

$$\boldsymbol{\pi}_{\alpha} = \gamma_{\alpha} m_{\alpha} \mathbf{v}_{\alpha} \quad (9.80)$$

is the relativistic *mechanical* momentum of particle number α , and

$$\mathbf{P}_{\text{trans}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{E}_T(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t) d^3r \quad (9.81)$$

is the momentum associated to the transverse part of the electromagnetic field. With reference to (9.79), it appears that

$$\mathbf{p}_{\alpha} = \boldsymbol{\pi}_{\alpha} + q_{\alpha} \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t) \quad (9.82)$$

may be considered as the total momentum of particle α . The vector $\mathbf{p}_{\alpha}$ is called the *canonical* (or *generalized*) momentum of the particle. In Part III, we shall realize that $\mathbf{p}_{\alpha}$ in the Coulomb gauge is the conjugate momentum to the particle position coordinate, $\mathbf{r}_{\alpha}$. In the framework of quantum mechanics, it is the momentum $\mathbf{p}_{\alpha}$ which translates into a momentum operator, i.e., $\mathbf{p}_{\alpha} \rightarrow (\hbar/i)\nabla_{\alpha}$ in the configuration space representation. The generalized momentum of a particle hence is the sum of its mechanical and electromagnetic momenta; see Fig. 9.2. A particle possesses an electromagnetic momentum part wherever in space the transverse vector potential is nonvanishing. This aspect of the theory manifests itself in a particularly pure

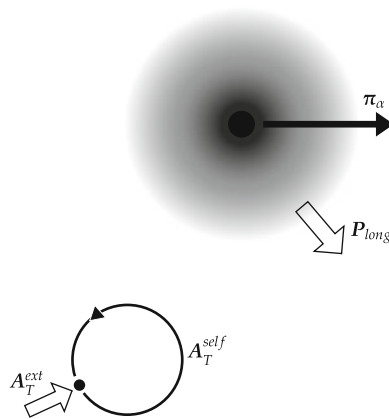


Fig. 9.2 *Top figure:* The generalized momentum of a charged particle (α) is the sum of its mechanical momentum ($\boldsymbol{\pi}_{\alpha}$) and the electromagnetic momentum ($\mathbf{P}_{\text{long}}$) associated with the transverse part of the vector potential ($\mathbf{A}_T(\mathbf{r}_{\alpha}(t), t)$) acting on the particle. The entire rim zone of the particle contributes to the electromagnetic momentum; cf. (9.72). *Bottom figure:* The transverse vector potential acting on the particle is the sum of the external potential ($\mathbf{A}_T^{\text{ext}}$) and the self-field potential ($\mathbf{A}_T^{\text{self}}$)

form if a charged particle (subscript α left out below) moves in a certain external (prescribed) transverse vector potential field, $\mathbf{A}_T^{\text{ext}}$. In addition to the particle's own generalized momentum given by $\boldsymbol{\pi} + q\mathbf{A}_T^{\text{self}}$, where $\mathbf{A}_T^{\text{self}}$ is the transverse vector potential generated by the particle itself (self-field), the particle requires a contribution $q\mathbf{A}_T^{\text{ext}}$ to its electromagnetic momentum from the prescribed external field. A physical effect on the particle thus may occur if the particle moves in a region of space where $\mathbf{A}_T^{\text{ext}} \neq \mathbf{0}$ even if both $\mathbf{E}_T^{\text{ext}}$ and $\mathbf{B}^{\text{ext}}$ are zero in this region. In the framework of quantum mechanics the physical significance of the vector potential $\mathbf{A}_T^{\text{ext}}$ in cases where $\mathbf{E}_T^{\text{ext}} = \mathbf{B}^{\text{ext}} = \mathbf{0}$ was pointed out originally by Bohm and Aharonov [277, 278], and first observed by Chambers [279]. The Aharonov–Bohm effect relates to the phase shift which occurs in the particle wave function if the particle is transported from one point to another in space along a given path C . The resulting phase shift is proportional to the line integral of the transverse vector potential along C between the initial and final positions. In a broader perspective, electromagnetic forces can be said to originate from the requirement that all observable effects in quantum mechanics should be independent of *local* phase transformations of the particle wave function. We shall return to the relation between electromagnetic forces and local phase invariance in Sect. 11.6.4.

9.3.4 Particle Angular Momentum Associated with the Longitudinal Electric Field

In analogy to the division of the field momentum introduced in the previous subsection, we define the longitudinal part of the angular momentum of the electromagnetic field, given in (2.104), by

$$\mathbf{I}_{\text{long}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{r} \times (\mathbf{E}_L(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r. \quad (9.83)$$

Using (9.39), and afterwards a well known expression for the double vector product $\mathbf{E}_L \times (\nabla \times \mathbf{A}_T)$, yield

$$\mathbf{I}_{\text{long}} = \epsilon_0 \int_{-\infty}^{\infty} \left[\sum_i E_{L,i} \mathbf{r} \times \nabla A_{T,i} - \mathbf{r} \times (\mathbf{E}_L \cdot \nabla) \mathbf{A}_T \right] d^3r, \quad (9.84)$$

where the summation is over $i = x, y, z$. To simplify (9.84) let us first use the relation

$$-\mathbf{r} \times (\mathbf{E}_L \cdot \nabla) \mathbf{A}_T = \mathbf{E}_L \times \mathbf{A}_T - (\mathbf{E}_L \cdot \nabla)(\mathbf{r} \times \mathbf{A}_T), \quad (9.85)$$

and let us thereafter integrate the last term in (9.85) by parts. This integration gives a surface integral at infinity. We shall assume that the fields go to zero so rapidly that this integral vanishes. Hence,

$$-\epsilon_0 \int_{-\infty}^{\infty} (\mathbf{E}_L \cdot \nabla)(\mathbf{r} \times \mathbf{A}_T) d^3r = \epsilon_0 \int_{-\infty}^{\infty} (\nabla \cdot \mathbf{E}_L)(\mathbf{r} \times \mathbf{A}_T) d^3r. \quad (9.86)$$

By combining (9.84)–(9.86) we have

$$\mathbf{I}_{\text{long}} = \epsilon_0 \int_{-\infty}^{\infty} \left[\sum_i E_{L,i} \mathbf{r} \times \nabla A_{T,i} + \mathbf{E}_L \times \mathbf{A}_T + (\nabla \cdot \mathbf{E}_L) \mathbf{r} \times \mathbf{A}_T \right] d^3r. \quad (9.87)$$

It appears from (9.52) that one always can write the longitudinal electric field as (minus) the gradient of a scalar function U , i.e.,

$$\mathbf{E}_L = -\frac{\partial \mathbf{A}_L}{\partial t} - \nabla \phi \equiv -\nabla U. \quad (9.88)$$

In the Coulomb gauge, where $\mathbf{A}_L = \mathbf{0}$, U equals the scalar potential ϕ . By insertion of (9.88) into the first two terms in (9.87), these become after partial integration, where surface terms at infinity again are assumed to vanish,

$$\begin{aligned} & \epsilon_0 \int_{-\infty}^{\infty} \left[\sum_i E_{L,i} \mathbf{r} \times \nabla A_{T,i} + \mathbf{E}_L \times \mathbf{A}_T \right] d^3r \\ &= \epsilon_0 \int_{-\infty}^{\infty} U \left[\sum_i \nabla_i (\mathbf{r} \times \nabla) A_{T,i} + \nabla \times \mathbf{A}_T \right] d^3r. \end{aligned} \quad (9.89)$$

Since

$$\begin{aligned} \sum_i \nabla_i (\mathbf{r} \times \nabla) A_{T,i} &= \sum_i (\nabla_i \mathbf{r}) \times \nabla A_{T,i} + \mathbf{r} \times \sum_i \nabla_i \nabla A_{T,i} \\ &= -\nabla \times \mathbf{A}_T + \mathbf{r} \times \nabla (\nabla \cdot \mathbf{A}_T) = -\nabla \times \mathbf{A}_T \end{aligned} \quad (9.90)$$

it is realized that the last expression in (9.89) is zero. Altogether, we thus obtain

$$\mathbf{I}_{\text{long}} = \int_{-\infty}^{\infty} \rho(\mathbf{r}, t) \mathbf{r} \times \mathbf{A}_T(\mathbf{r}, t) d^3r, \quad (9.91)$$

since $\epsilon_0 \nabla \cdot \mathbf{E}_L = \rho$. For an assembly of point charges, we hence have realized that

$$\mathbf{I}_{\text{long}} = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha}(t) \times \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t). \quad (9.92)$$

For each particle α in the assembly we may thus introduce a generalized particle angular momentum

$$\mathbf{r}_{\alpha} \times \mathbf{p}_{\alpha} = \mathbf{r}_{\alpha} \times (\boldsymbol{\pi}_{\alpha} + q_{\alpha} \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t)), \quad (9.93)$$

cf. (2.103) (with $\mathbf{p}_\alpha$ replaced by $\boldsymbol{\pi}_\alpha$) and (9.92). The total angular momentum of the global field–particle system hence may be written in the physically appealing form

$$\mathbf{I} = \sum_{\alpha} \mathbf{r}_{\alpha} \times (\boldsymbol{\pi}_{\alpha} + q_{\alpha} \mathbf{A}_T(\mathbf{r}_{\alpha}(t), t)) + \mathbf{I}_{\text{trans}}, \quad (9.94)$$

where

$$\mathbf{I}_{\text{trans}} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{r} \times (\mathbf{E}_T(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3 r \quad (9.95)$$

is the angular momentum associated to the transverse part of the electromagnetic field, so to speak.

9.4 Dynamical State of the Coupled Field–Particle System

The microscopic Maxwell–Lorentz equations (2.1)–(2.4) show that the evolution of the electromagnetic field in space-time depends on the particle dynamics through the charge (ρ) and current ($\mathbf{J}$) densities. For point-particles these densities are given in terms of the position ($\mathbf{r}_{\alpha}$) and velocity ($\mathbf{v}_{\alpha}$) of the various (α) particles, and the charges of these, of course; see (2.28) and (2.29). The particle dynamics is determined via the (relativistic) Newton–Lorentz equations for the different particles (2.30). The motion of the individual particles depends on the electric ($\mathbf{E}(\mathbf{r}_{\alpha}(t), t)$) and magnetic ($\mathbf{B}(\mathbf{r}_{\alpha}(t), t)$) fields at the particle positions. The microscopic Maxwell–Lorentz equations and the Newton–Lorentz equations form two sets of coupled equations. At a given time, say $t = t_0$, the global state of the coupled field–particle system is specified giving the electric and magnetic fields at all points ($\mathbf{r}$) in space and the position and velocity of each particle, i.e.,

$$[\mathbf{E}(\mathbf{r}, t_0), \mathbf{B}(\mathbf{r}, t_0), \{\mathbf{r}_{\alpha}(t_0)\}, \{\mathbf{v}_{\alpha}(t_0)\}]. \quad (9.96)$$

Since the analysis in this section has shown that the longitudinal part of the electric field can be expressed exclusively in terms of the particle position variables $\{\mathbf{r}_{\alpha}(t_0)\}$, see (9.54), the state of the global field–particle system is completely specified at $t = t_0$ by giving

$$[\mathbf{E}_T(\mathbf{r}, t_0), \mathbf{B}(\mathbf{r}, t_0), \{\mathbf{r}_{\alpha}(t_0)\}, \{\mathbf{v}_{\alpha}(t_0)\}] \quad (9.97)$$

for all $\mathbf{r}$ -points and all α . The transverse electric field and the magnetic fields are not independent of each other but coupled directly via $\nabla \times \mathbf{E}_T = -\partial \mathbf{B} / \partial t$, and this enables one to improve the specification of the dynamical state at $t = t_0$ further. We shall discuss certain choices of improvement in connection to (1) the theory of photon wave mechanics, and (2) QED (quantum optics).

Chapter 10

Linear Nonlocal Response Theory

10.1 Response Theory for Transverse External Excitations

10.1.1 Many-Body Constitutive Relation

Let us assume that we have two groups of (charged) particles in motion and separated so far from each other that the rim zones of the groups do not overlap (significantly) in space. In such a case, the electromagnetic coupling between the particles of the two groups is brought about only by the transverse part of the electromagnetic field, cf. the discussion in Sects. 9.2.1 and 9.2.2. In general (inevitably), the coupling goes both ways, but in many cases it can with sufficient accuracy be assumed that the coupling is a one-way coupling, and it is in these cases that response theory can be introduced. If, for instance, the field of a laser beam interacts with a microscopic or mesoscopic object it can usually be assumed that the motion of the particles in the laser cavity is unaffected by the electromagnetic field emitted from the object in response to the incoming laser field. In this case, the one group of particles consists of the particles in the laser cavity, and the other group is formed by the particles of our microscopic or mesoscopic object, and the coupling is a one-way coupling to which response theory always can be applied. If the object under study is, say, a metallic mirror oriented in such a manner in space that the laser light hitting the mirror is reflected back into the laser cavity the field-matter interaction inside the cavity will be modified, and response theory cannot, at least in general, be applied to this situation. In the following it is assumed that the electromagnetic coupling is a one-way coupling. The particles constituting the one group will be called the source particles, and it is the dynamics of these particles we assume develops independently of the field generated by the motions of the particles in the other group. The transverse electric field generated by the source particles is called the external field, and it is denoted by $\mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$ below. The external field induces a motion in the other group (the system particles), and this motion itself generates an electromagnetic field inside (and outside) the system under study. The resulting (prevailing) transverse electric field we denote by $\mathbf{E}_T(\mathbf{r}, t)$.

In *linear* response theory it is assumed that the current density, $\mathbf{J}(\mathbf{r}, t)$, induced by the prevailing (local) transverse electric field is linearly related to this field, i.e.,

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') dt' d^3 r'. \quad (10.1)$$

If the external field $\mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$ is weak it is often correct to assume that the relation between $\mathbf{J}$ and $\mathbf{E}_T$ is linear. The second rank tensor $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t')$ is here called the microscopic linear conductivity tensor, or just the conductivity tensor. The relation in (10.1), often called a constitutive relation, connects the induced current density at a given point ($\mathbf{r}$) in space not only to the transverse electric field at the same point but also to the transverse field in the neighbourhood ($\mathbf{r}' \neq \mathbf{r}$); see Fig. 10.1. In near-field electrodynamics it is important that this *spatial nonlocality* is kept in the constitutive equation. The coupling between $\mathbf{J}(\mathbf{r}, t)$ and $\mathbf{E}_T(\mathbf{r}', t')$ is also *nonlocal in time* ($t \neq t'$). As indicated in (10.1), the linear conductivity tensor $\boldsymbol{\Sigma}$ thus is a function of $\mathbf{r}, \mathbf{r}', t$ and t' in the most general situation.

The constitutive relation in (10.1) is *not* causal in the sense that the current density $\mathbf{J}(\mathbf{r}, t)$ at time $t = t$ only depends on the transverse electric field $\mathbf{E}_T(\mathbf{r}', t')$ prevailing at the various $\mathbf{r}'$ positions at earlier times ($t' < t$). The reason for this lack of causality is associated to the fact that it is the prevailing (local) field $\mathbf{E}_T(\mathbf{r}', t')$ and *not* the externally impressed field $\mathbf{E}_T^{\text{ext}}(\mathbf{r}', t')$ which enters (10.1). We shall have more to say on this below.

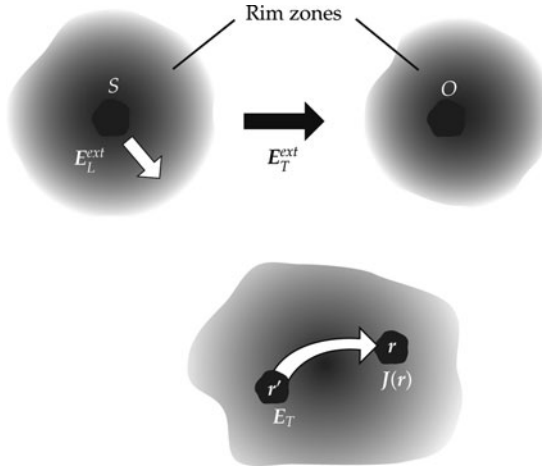


Fig. 10.1 *Top figure:* A source particle (S) emits a prescribed (external) transverse electric field ($\mathbf{E}_T^{\text{ext}}$), and generates also a longitudinal electric field ($\mathbf{E}_L^{\text{ext}}$) in its rim zone. Another particle (O) responds to the field of S . Only the transverse part of the external field drives the dynamics of O when the two particles are not in rim-zone contact. *Bottom figure:* The microscopic current density ($\mathbf{J}$) at a given point ($\mathbf{r}$) in space is determined by the transverse part of the local electric field ($\mathbf{E}_T$) in neighboring points ($\mathbf{r}'$). The spatial range of the connection between $\mathbf{E}_T(\mathbf{r}', t')$ and $\mathbf{J}(\mathbf{r}, t)$ is determined by the nonlocal correlation range hidden in the microscopic conductivity tensor $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t')$. The domain of nonvanishing $\boldsymbol{\Sigma}$ is indicated in light grey tone

When the transverse external field, $\mathbf{E}_T^{\text{ext}}$, acts on our mesoscopic (or microscopic) system the induced motion of the particles will give rise to the presence of both transverse, $\mathbf{E}_T$, and longitudinal, $\mathbf{E}_L$, time dependent local electric fields, so why does the longitudinal part of the local field not enter the constitutive relation? The answer to this question relates to the fact that the longitudinal electric field is *not* a true dynamical variable (see Sect. 9.4). When $\mathbf{E}_L$ is eliminated in favour of the particle position variables $\{\mathbf{r}_\alpha(t)\}$ (see (9.54)) the role of the longitudinal field appears via the solution of the many-body Schrödinger equation used to determine the microscopic conductivity tensor; see Chap. 11.

10.1.2 Integral Equation for the Transverse Electric Field

By means of the transverse delta function the transverse part of the current density in (10.1) can be determined. Thus, one has

$$\mathbf{J}_T(\mathbf{r}, t) = \int_{-\infty}^{\infty} \boldsymbol{\Sigma}_T(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') dt' d^3r', \quad (10.2)$$

where

$$\boldsymbol{\Sigma}_T(\mathbf{r}, \mathbf{r}', t, t') = \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}'') \cdot \boldsymbol{\Sigma}(\mathbf{r}'', \mathbf{r}', t, t') d^3r''. \quad (10.3)$$

An integral equation for the unknown local electric field $\mathbf{E}_T(\mathbf{r}, t)$ now can be established by combination of (9.30) and (10.2). From (9.30) the following integral expression for $\mathbf{E}_T(\mathbf{r}, t)$ may be obtained:

$$\mathbf{E}_T(\mathbf{r}, t) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t) - \mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \frac{\partial}{\partial t'} \mathbf{J}_T(\mathbf{r}', t') dt' d^3r'. \quad (10.4)$$

That the integral in (10.4) represents the physically correct particular solution to (9.30) follows directly from (2.14) and (2.16) and the discussion given in Sect. 2.3. By insertion of (10.2) into (10.4) one gets an inhomogeneous integral equation for the transverse part of the electric field, viz.,

$$\mathbf{E}_T(\mathbf{r}, t) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t) + \int_{-\infty}^{\infty} \mathbf{K}_T(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') dt' d^3r'. \quad (10.5)$$

The kernel of the integral equation,

$$\mathbf{K}_T(\mathbf{r}, \mathbf{r}', t, t') = -\mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}''|, t - t'') \cdot \frac{\partial}{\partial t''} \boldsymbol{\Sigma}_T(\mathbf{r}'', \mathbf{r}', t'', t') dt'' d^3r'', \quad (10.6)$$

is a folding integral in space–time of the Huygens propagator and the time derivative of the microscopic conductivity tensor $\boldsymbol{\Sigma}_T$.

10.1.3 Causal Response Tensors: Microscopic Conductivity

The formal solution to (10.5),

$$\mathbf{E}_T(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3r', \quad (10.7)$$

gives an integral relation between the transverse parts of the local and external electric fields. The kernel $\mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t')$ hence is called the transverse local-field tensor. Since the contribution $d\mathbf{E}_T(\mathbf{r}, t)$ to the local field at the arbitrary point $\mathbf{r}$ from the externally impressed field in an infinitesimal volume d^3r' centered at $\mathbf{r}'$ cannot precede $\mathbf{E}_T^{\text{ext}}(\mathbf{r}', t')$ in time, the local-field tensor is a causal response tensor satisfying the condition

$$\mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t'(> t)) = \mathbf{0}. \quad (10.8)$$

By substitution of (10.7) into (10.5) it appears that the transverse local-field tensor satisfies the integral equation

$$\begin{aligned} \mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t') &= \mathbf{U} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \\ &+ \int_{-\infty}^{\infty} \mathbf{K}_T(\mathbf{r}, \mathbf{r}'', t, t'') \cdot \mathbf{L}_T(\mathbf{r}'', \mathbf{r}', t'', t') dt'' d^3r''. \end{aligned} \quad (10.9)$$

From a knowledge of the transverse local-field tensor the current density response $\mathbf{J}(\mathbf{r}, t)$ to the externally impressed and prescribed transverse electric field $\mathbf{E}_T^{\text{ext}}(\mathbf{r}', t')$ can be obtained from the constitutive equation

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3r', \quad (10.10)$$

where the kernel

$$\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}', t, t') = \int_{-\infty}^{\infty} \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'', t, t'') \cdot \mathbf{L}_T(\mathbf{r}'', \mathbf{r}', t'', t') dt'' d^3r'' \quad (10.11)$$

is called the causal microscopic conductivity tensor, because

$$\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}', t, t'(> t)) = \mathbf{0} \quad (10.12)$$

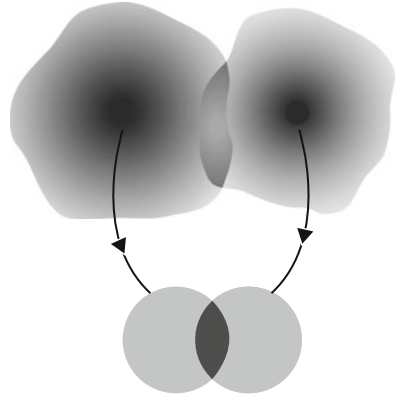
for all pairs of $(\mathbf{r}, \mathbf{r}')$ -points.

10.2 Causality and Dispersion Relations

10.2.1 Einstein Causality and Microcausality

The notion of causality involves a time ordering in the sense that what we call *cause* must always precede the *effect*. The causality concept is however rather useless in physics unless a precise definition is given of the words *cause* and *effect*. In the framework of microscopic classical electrodynamics it is fruitful to relate these words to the time dependent motions of the charged particles. In the Maxwell–Lorentz equations, these motions are described in terms of the prevailing current density distribution $\mathbf{J}(\mathbf{r}, t)$. The concepts *cause* and *effect* now make sense if a certain division of the charge density distribution $\rho(\mathbf{r}, t)$ can be made. Thus, let us assume that $\rho(\mathbf{r}, t)$ can be divided into two *spatially separated* distributions, and that all the particles are at rest in a certain inertial system up to the time $t = t_0$. Let us further assume that the rim zones of the two distributions do not overlap at any time during the charge movement. Let us now imagine that the charges in one of the groups are set in motion at $t = t_0$, and let us denote the generated current density distribution by $\mathbf{J}^{\text{cause}}(\mathbf{r}, t)$. This current density distribution in turn generates an electromagnetic field whose electric part we denote by $\mathbf{E}^{\text{cause}}(\mathbf{r}, t)$. The transverse part, $\mathbf{E}_T^{\text{cause}}(\mathbf{r}, t)$, of this field spreads out in space with the vacuum speed of light, and after a certain (finite) time the transverse electromagnetic field reaches the other group of particles and sets these in motion. The induced current density distribution we denote by $\mathbf{J}^{\text{effect}}(\mathbf{r}, t)$. A causality concept can in a meaningful manner thus be attached to the *cause*, $\mathbf{J}^{\text{cause}}(\mathbf{r}, t)$, and the *effect*, $\mathbf{J}^{\text{effect}}(\mathbf{r}, t)$, and one may call this kind of causality for *Einstein causality* because the *cause* precedes the *effect* with the time it takes for the transverse electromagnetic field to propagate (with the speed c_0) between the two particle distributions. If the two charge distributions were placed so close to each other that the respective rim zones overlap the situation would be more complicated for two reasons. Firstly, it would be difficult (if not impossible!) to excite at $t = t_0$ the one group of particles without affecting simultaneously particles in the other group. This is so because a third group of particles (or at least one particle) is needed in the first instance to make the electromagnetic excitation at $t = t_0$, and one must imagine this excitation to be so localized in space that it only affects the one group of charges. Since, as we shall realize in Chaps. 14 and 18, it is in general impossible to localize electromagnetic fields better in space than to regions of near-field dimensions it is not easy to imagine an excitation at $t = t_0$ of only the one group of particles. Secondly, a time dependent longitudinal electric field would be set up between the two groups of charges, and it is not easy to introduce a causality concept in this situation in view of the fact that the longitudinal electric field (which relates to an instantaneous Coulomb interaction) is not a dynamical variable (Fig. 10.2). We shall have more to say on the longitudinal field interaction later on in this book since this kind of interaction plays a particular role in near-field electrodynamics, not least in a quantum physical context.

Fig. 10.2 Two particles in rim-zone contact. The spatial overlap of the longitudinal electric fields of the particles makes a strict causal description of the particle–particle interaction impossible long before the particles come in electronic contact (lower part of the figure)



In relation to (10.10) a somewhat different meaning is associated with the word causality. Thus, the *cause* is the transverse part of the external electric field, $E_T^{\text{ext}}(\mathbf{r}, t)$, and the *effect* is the current density, $\mathbf{J}(\mathbf{r}, t)$, in the system (atom, molecule, mesoscopic object,...) under study. The external field is generated by the current density $\mathbf{J}^{\text{ext}}(\mathbf{r}, t)$ of an external group of charges, and this current density corresponds to $\mathbf{J}^{\text{cause}}(\mathbf{r}, t)$ introduced above. An Einstein causal connection therefore exists between $\mathbf{J}^{\text{ext}}(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$. The relation between $E_T^{\text{ext}}(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ is causal in the sense of (10.12), but not necessarily Einstein causal, because a quantum physical determination of the conductivity $\sigma(\mathbf{r}, \mathbf{r}', t, t')$ is required in general. So-called nonlocal quantum effects appear in the expression for $\sigma(\mathbf{r}, \mathbf{r}', t, t')$, and these effects do not obey the restrictive Einstein causality criterion. In a quantum physical context the condition in (10.12) represents what one may call a microcausal relation between E_T^{ext} and $\mathbf{J}$ in (10.10). The transverse local-field tensor $L_T(\mathbf{r}, \mathbf{r}', t, t')$ satisfies the causal condition in (10.8), and this leads to microcausality between E_T^{ext} and E_T in (10.7).

10.2.2 Causality and Analyticity: Translational Invariance in Time

The absence of advanced effects in physics leads to the existence of certain so-called microscopic frequency dispersion relations, as we shall realize below in the context of linear response theory. These dispersion relations are important not only in answering important and deep questions in (quantum) electrodynamics, but also because a variety of other macroscopic dispersion relations of great practical use in electrodynamics can be derived from the microscopic ones. We shall illustrate the main principles via a study of the constitutive relation given in (10.10).

To lighten the notation in the subsequent analysis, the dependence of the causal microscopic conductivity tensor on the space coordinates $\mathbf{r}$ and $\mathbf{r}'$ will

be suppressed, and the abbreviation

$$\sigma(\mathbf{r}, \mathbf{r}', t, t') = \sigma(t, t') \quad (10.13)$$

is used. In order to derive the aforementioned dispersion relations we make a Fourier integral transformation of $\sigma(t, t')$ in the time coordinate t' , that is

$$\sigma(t, t') = (2\pi)^{-1} \int_{-\infty}^{\infty} s(t; \omega) e^{-i\omega(t-t')} d\omega, \quad (10.14)$$

where

$$s(t; \omega) = \sigma(t; \omega) e^{i\omega t}. \quad (10.15)$$

In the transformation above, a factor $\exp(+i\omega t')$ is used instead of the usual factor $\exp(-i\omega t')$. Formally, we now replace the real frequency ω in (10.14) by a complex frequency, also denoted by $\omega (= \Re\omega + i\Im\omega)$. As we shall realize now, the causality criterion in (10.12) will be fulfilled if $s(t; \omega)$ is an analytic function in the upper half ($\Im\omega > 0$) of the complex ω -plane, and on the real axis. Since $\exp[-i\omega(t-t')]$ is an analytic function of ω the assumed analyticity of $s(t; \omega)$ implies that the integral of $s(t; \omega)\exp[-i\omega(t-t')]$ along an arbitrary closed contour C in the upper half plane (including the real axis) will vanish, i.e.,

$$\oint_C s(t; \omega) e^{-i\omega(t-t')} d\omega = 0. \quad (10.16)$$

If the contour consists of a semicircle, which radius we let go to infinity, plus, in the limit, the entire real axis, the integral over the semicircle will vanish for $t' > t$ since $\exp[(t-t')\Im\omega]$ goes exponentially fast to zero, and *provided* $s(t; \omega)$, in case, does not grow too fast for $|\omega| \rightarrow \infty$. For the systems of interest in this book, the integral over the semicircle always vanishes in the limit $|\omega| \rightarrow \infty$. From (10.16) it then appears that the integral along the real axis in (10.14) is zero for $t' > t$. The opposite is also true, namely that the causality criterion in (10.12) implies that the function $s(t; \omega)$ must be analytic in the upper half of the complex ω -plane.

If the physical properties of the medium under study (or at least those properties which are of interest electrodynamically) do not change over time, the various linear response tensors ($\boldsymbol{\Sigma}$, $\mathbf{L}_T$, σ , etc.) cannot depend on t and t' separately, but only on the difference $t - t'$. In the case of the causal microscopic conductivity tensor, translational invariance in time means that

$$\sigma(\mathbf{r}, \mathbf{r}', t, t') = \sigma(\mathbf{r}, \mathbf{r}', t - t'), \quad (10.17)$$

and in consequence the spatially and temporarily nonlocal constitutive equation

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \sigma(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3r' \quad (10.18)$$

is reduced to the form

$$\mathbf{J}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}'; \omega) d^3 r' \quad (10.19)$$

in the space–frequency domain. For media exhibiting translational invariance in time excitation by a monochromatic external field will generate a current density distribution oscillating at precisely the incoming frequency in the framework of linear response theory. When (10.17) is satisfied a comparison of the Fourier integral

$$\boldsymbol{\sigma}(t - t') = (2\pi)^{-1} \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\omega) e^{-i\omega(t-t')} d\omega, \quad (10.20)$$

to the one in (10.14) shows that

$$s(t; \omega) = \boldsymbol{\sigma}(\omega) \quad (10.21)$$

for media with time invariant physical properties. The analytic function s is therefore time independent for such media.

10.2.3 Frequency Dispersion and Hilbert Transforms

Restricting ourselves to media exhibiting translational invariance in time, let us now consider the contour integral

$$\mathbf{I}(\omega_0) = \oint_C \frac{\boldsymbol{\sigma}(\omega)}{\omega - \omega_0} d\omega, \quad (10.22)$$

where $\boldsymbol{\sigma}(\omega) \equiv \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ is the causal microscopic linear conductivity tensor (an analytic function in the upper half ($\Im \omega \geq 0$) of the complex ω -plane), and ω_0 is a real ($-\infty < \omega_0 < \infty$) angular frequency. The integral in (10.22) thus has a first-order pole on the real axis at $\omega = \omega_0$. For a closed contour (C) located entirely in the upper half plane Cauchy's integral theorem implies that $\mathbf{I}(\omega_0) = \mathbf{0}$. Let us now choose a contour C consisting of the following pieces: (1) A semicircle of radius R and with center at the origin of the complex plane, (2) a straight-line section along the real axis from $-R$ to $\omega_0 - \epsilon$, (3) a semicircle centered on ω_0 and of radius ϵ , and (4) a straight-line section along the real axis from $\omega_0 + \epsilon$ to R (see Fig. 10.3). We integrate the contour in the counter-clockwise direction and take the limits $R \rightarrow \infty$ and $\epsilon \rightarrow 0$. In the limit $R \rightarrow \infty$ the contribution to the integral from the “big” semicircle vanishes, and the contribution from the “small” semicircle equals $-\pi i \boldsymbol{\sigma}(\omega_0)$ in the limit $\epsilon \rightarrow 0$. The sum of the two straight-line sections gives the principal value of the integral $\int_{-\infty}^{\infty} [\boldsymbol{\sigma}(\omega)/(\omega - \omega_0)] d\omega$ in the limits $R \rightarrow \infty$, $\epsilon \rightarrow 0$. Altogether, one thus has obtained for real ω the result

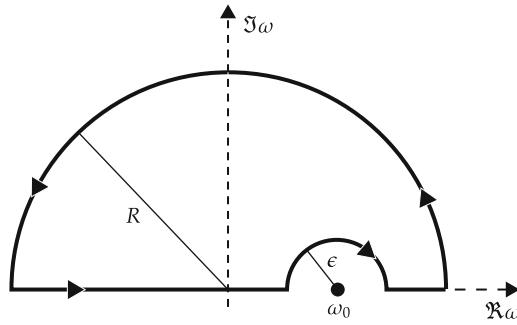


Fig. 10.3 Schematic illustration of the contour which in a complex frequency (ω) plane is used to establish the Kramers–Kroening relations between the real and imaginary parts of the *causal* microscopic linear conductivity tensor. The first-order pole in the relevant contour integral is located on the real axis at ω_0 . The radii of the two semicircles take on the limiting values $R \rightarrow \infty$ and $\epsilon \rightarrow 0$ by the end of the calculation

$$P \int_{-\infty}^{\infty} \frac{\sigma(\omega)}{\omega - \omega_0} d\omega = \pi i \sigma(\omega_0), \quad (10.23)$$

where P stands for *principal value*. The causal conductivity tensor cannot be a real, nor a purely imaginary function of ω if (10.23) is to be satisfied. If one divides the conductivity tensor into its real ($\Re$) and imaginary ($\Im$) parts, i.e.,

$$\sigma(\omega) = \Re\sigma(\omega) + i \Im\sigma(\omega), \quad (10.24)$$

Equation (10.23) immediately gives the following integral relations between the two parts:

$$\Re\sigma(\omega_0) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\Im\sigma(\omega)}{\omega - \omega_0} d\omega, \quad (10.25)$$

and

$$\Im\sigma(\omega_0) = \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{\Re\sigma(\omega)}{\omega - \omega_0} d\omega. \quad (10.26)$$

The real and imaginary parts of the causal conductivity (tensor) constitute a pair of Hilbert transforms. In physics, the real and imaginary parts of the frequency representative of any causal response function will form a pair of Hilbert transforms since causality implies analyticity in the upper half of the complex frequency plane. The integral relations in (10.25) and (10.26) (and equivalent ones for other causal response functions) often goes under the name Kramers–Kroening relations because quite similar relations, yet less general, were established originally independently by Kramers [205] and Kroenig [204]. The relations are also often in optics named (frequency) dispersion relations [53], and their great importance is partially related to the fact that the knowledge of either the real or imaginary part of the response function for all frequencies in principle allows one to determine the frequency dependence of the other one. It is often useful to limit the integrations in (10.25)

and (10.26) to only positive frequencies. The causal conductivity tensor is a real quantity in the space–time domain since it connects two real vector fields ($\mathbf{J}(\mathbf{r}, t)$ and $\mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$); see (10.18). According to (3.2) this implies that $\boldsymbol{\sigma}(-\omega) = \boldsymbol{\sigma}^*(\omega)$, or equivalently $\Re\boldsymbol{\sigma}(-\omega) = \Re\boldsymbol{\sigma}(\omega)$ and $\Im\boldsymbol{\sigma}(-\omega) = -\Im\boldsymbol{\sigma}(\omega)$. Using the last two relations it is easy to show that

$$P \int_{-\infty}^0 \frac{\Im\boldsymbol{\sigma}(\omega)}{\omega - \omega_0} d\omega = P \int_0^{\infty} \frac{\Im\boldsymbol{\sigma}(\omega)}{\omega + \omega_0} d\omega, \quad (10.27)$$

and

$$P \int_{-\infty}^0 \frac{\Re\boldsymbol{\sigma}(\omega)}{\omega - \omega_0} d\omega = -P \int_0^{\infty} \frac{\Re\boldsymbol{\sigma}(\omega)}{\omega + \omega_0} d\omega. \quad (10.28)$$

If the negative frequency parts of the integrals in (10.25) and (10.26) are replaced by the positive-frequency expression in (10.27) and (10.28) one obtains the desired dispersion relations, viz.,

$$\Re\boldsymbol{\sigma}(\omega_0) = \frac{2}{\pi} P \int_0^{\infty} \frac{\omega \Im\boldsymbol{\sigma}(\omega)}{\omega^2 - \omega_0^2} d\omega, \quad (10.29)$$

and

$$\Im\boldsymbol{\sigma}(\omega_0) = -\frac{2}{\pi} P \int_0^{\infty} \frac{\omega_0 \Re\boldsymbol{\sigma}(\omega)}{\omega^2 - \omega_0^2} d\omega. \quad (10.30)$$

In finishing this section it is important to emphasize that the conductivity tensor $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t') = \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t - t')$ (for systems translationally invariant in time) *does not* satisfy dispersion relation of the forms given in (10.25) and (10.26) since $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t - t')$ is not a causal response tensor.

10.3 Local and Near-Local Microscopic Response Tensors

10.3.1 Spatial Correlation Range in Constitutive Equations

The starting point for the preceding microscopic analyses of the linear particle response to transverse field excitations was the constitutive equation in Sect. 10.1. Under which circumstances is it important to keep the spatial nonlocality between the current density and the transverse part of the local electric field in microscopic response theory? To investigate this question it is sufficient to limit ourselves to media exhibiting translational invariance in time, so that $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t') = \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t - t')$. In the space–frequency domain (10.1) then takes the form

$$\mathbf{J}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T(\mathbf{r}'; \omega) d^3 r'. \quad (10.31)$$

In principle, the response tensor $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$ can be determined via a quantum mechanical many-body calculation. We shall undertake such a calculation in Chap. 11, and it will appear from this that the spatial range over which $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$ couples $\mathbf{J}(\mathbf{r}; \omega)$ and $\mathbf{E}_T(\mathbf{r}; \omega)$ is of the order of the range of the many-body transition current densities involved when the medium is excited by the transverse local field $\mathbf{E}_T$. One may call this range the correlation range of the response tensor ($\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$). To judge the importance of the spatial nonlocality in (10.31) the length scale on which typical variations in $\mathbf{E}_T(\mathbf{r}; \omega)$ occurs must be known. The spatial variations in $\mathbf{E}_T(\mathbf{r}; \omega)$ can be estimated from the space–frequency representative of (10.4), i.e.,

$$\mathbf{E}_T(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + i\mu_0\omega \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r'. \quad (10.32)$$

The spatial variations in $\mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega)$ are determined by the transverse current density distribution $\mathbf{J}_T^{\text{ext}}(\mathbf{r}'; \omega)$ of the source particles and the distance of the source from the medium under study. With no loss of generality one may assume that the external source is so far from our medium that $\mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega)$ does not vary across our medium. The spatial variation of $\mathbf{E}_T(\mathbf{r}; \omega)$ over the correlation range of $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$ thus is determined by the variation with $\mathbf{r}$ of the integral term in (10.32). The variation of this term is related to the variations in the integral of the Huygens propagator $g(|\mathbf{r} - \mathbf{r}'|; \omega)$ over a volume of the same linear extension as the actual rim zone of our medium, cf. the same discussion in Sect. 9.2. If the correlation range in $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$ therefore is much smaller than the linear extension of the rim zone the spatial variations in the transverse field $\mathbf{E}_T(\mathbf{r}'; \omega)$ over the correlation range can in general be neglected. Since the correlation range in $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$ quantitatively speaking never exceeds the electronic size of the medium (in many cases it is much smaller), the spatial nonlocality in (10.31) in general will be negligible for a mesoscopic object of linear extension much smaller than that of its rim zone. The insensitivity of the integral in (10.32) to small variations in $\mathbf{r}$ relates to the fact that the integral has no contribution from the neighborhood of the singular point $\mathbf{r}' = \mathbf{r}$. To prove this let us consider the contribution from a small spherical volume, $v(\epsilon)$, centered on $\mathbf{r}$ and of radius ϵ . For sufficiently small ϵ one has

$$\int_{v(\epsilon)} g(R; \omega) \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' \approx \left[\int_{v(\epsilon)} g(R; \omega) d^3 r' \right] \mathbf{J}_T(\mathbf{r}; \omega), \quad (10.33)$$

and it is easy to show that the integral over the quasi-static Huygens propagator $g(R; \omega) \approx 4\pi|\mathbf{r} - \mathbf{r}'|^{-1}$ is proportional to ϵ^2 in the limit $\epsilon \rightarrow 0$. Since the integral over an $|\mathbf{r} - \mathbf{r}'|^{-1}$ singularity is absolutely convergent the small integration volume need not be a sphere, the sphere just makes the calculation easy (in spherical coordinates).

Let us now turn the attention towards the linear constitutive equation involving the causal microscopic conductivity tensor. In media exhibiting translational invariance in time so that $\sigma(\mathbf{r}, \mathbf{r}', t, t') = \sigma(\mathbf{r}, \mathbf{r}', t - t')$ the equation takes the form given

in (10.19) in the space–frequency domain. For an easy comparison to (10.31) let us repeat (10.19) here:

$$\mathbf{J}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}'; \omega) d^3 r'. \quad (10.34)$$

Since the transverse part of the external field usually varies much more slowly in space than the transverse part of the local electric field in the medium, the reader might be tempted to believe immediately that the spatial nonlocality inherent in (10.34) will be unimportant in most cases. Before we possibly draw such a conclusion let us compare the correlation ranges of the response tensors $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ and $\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega)$. Since the transverse local-field tensor also must have the form $\mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t') = \mathbf{L}_T(\mathbf{r}, \mathbf{r}', t - t')$ in the present case, insertion of Fourier integral transforms for $\boldsymbol{\sigma}$, $\boldsymbol{\Sigma}$, and $\mathbf{L}_T$ in (10.11) results in the following spatially nonlocal relation between $\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ and $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'; \omega)$:

$$\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) = \int_{-\infty}^{\infty} \boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}''; \omega) \cdot \mathbf{L}_T(\mathbf{r}'', \mathbf{r}'; \omega) d^3 r''. \quad (10.35)$$

It appears from (the space–frequency representation of) (10.9) that $\mathbf{L}_T(\mathbf{r}, \mathbf{r}'; \omega)$ and $\mathbf{K}_T(\mathbf{r}, \mathbf{r}'; \omega)$ qualitatively have the same correlation range, and it further appears from (10.6) that the same holds for $\mathbf{K}_T(\mathbf{r}, \mathbf{r}'; \omega)$ and $\boldsymbol{\Sigma}_T(\mathbf{r}'', \mathbf{r}'; \omega)$. Since the correlation range of $\boldsymbol{\Sigma}_T(\mathbf{r}'', \mathbf{r}'; \omega)$ equals the range of the rim zone, (10.3), it follows that the correlation range in $\mathbf{L}_T(\mathbf{r}, \mathbf{r}'; \omega)$ is comparable to the extension of the rim zone. Altogether, it can thus be concluded from (10.35) that the correlation range of the causal conductivity tensor in (10.34) has the magnitude of the rim zone extension. The nonlocality in the constitutive relation between $\mathbf{J}(\mathbf{r}; \omega)$ and $\mathbf{E}_T^{\text{ext}}(\mathbf{r}'; \omega)$ must, therefore, be kept in cases where the transverse part of the external field varies appreciably over the rim zone volume.

10.3.2 Local Dynamics with Hidden Nonlocality

If the transverse external electric field varies slowly in space across the rim zone it is convenient to make a Taylor series expansion of $\mathbf{E}_T^{\text{ext}}(\mathbf{r}'; \omega)$ in (10.34) around $\mathbf{r}$, i.e.,

$$\mathbf{E}_T^{\text{ext}}(\mathbf{r}'; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + (\mathbf{r}' - \mathbf{r}) \cdot \nabla \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + \cdots. \quad (10.36)$$

In lowest order the constitutive relation takes the spatially local form

$$\mathbf{J}(\mathbf{r}; \omega) = \boldsymbol{\sigma}^l(\mathbf{r}; \omega) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega), \quad (10.37)$$

where

$$\boldsymbol{\sigma}^l(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) d^3 r' \quad (10.38)$$

is an effectively local (l) causal microscopic conductivity tensor. I call it *effectively* local because it is obtained via integration of the nonlocal conductivity tensor over the correlation volume of $\sigma(\mathbf{r}, \mathbf{r}'; \omega)$. The σ^l -tensor thus possesses what may be called hidden nonlocality.

10.4 Microscopic “Polarization” and “Magnetization” Dynamics

10.4.1 Generalized Polarization and Magnetization Concepts

Within the framework of the response theory approximation it is meaningful to divide the total (superscript tot) current and charge densities appearing in the microscopic Maxwell–Lorentz equations into two parts, i.e.,

$$\mathbf{J}^{\text{tot}}(\mathbf{r}, t) = \mathbf{J}^{\text{ext}}(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t), \quad (10.39)$$

$$\rho^{\text{tot}}(\mathbf{r}, t) = \rho^{\text{ext}}(\mathbf{r}, t) + \rho(\mathbf{r}, t). \quad (10.40)$$

The so-called external parts $\mathbf{J}^{\text{ext}}(\mathbf{r}, t)$ and $\rho^{\text{ext}}(\mathbf{r}, t)$ are assumed to be prescribed quantities related by the equation of continuity $\nabla \cdot \mathbf{J}^{\text{ext}} + \partial \rho^{\text{ext}} / \partial t = 0$. The parts $\mathbf{J}(\mathbf{r}, t)$ and $\rho(\mathbf{r}, t)$ belong to the system of particles which selfconsistent dynamics we want to study when driven by the external electromagnetic field ($\mathbf{E}^{\text{ext}} = \mathbf{E}_T^{\text{ext}} + \mathbf{E}_L^{\text{ext}}$, $\mathbf{B}^{\text{ext}} = \mathbf{B}_T^{\text{ext}}$) generated by $\mathbf{J}^{\text{ext}}$ and ρ^{ext} .

Let us now divide the microscopic current density $\mathbf{J}(\mathbf{r}, t)$ into two parts in the following manner:

$$\mathbf{J}(\mathbf{r}, t) \equiv \frac{\partial \mathbf{P}(\mathbf{r}, t)}{\partial t} + \nabla \times \mathbf{M}(\mathbf{r}, t). \quad (10.41)$$

In a somewhat indirect way two new microscopic vector fields $\mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t)$ are hereby introduced. These local fields are usually called the generalized (or microscopic) polarization ($\mathbf{P}(\mathbf{r}, t)$) and magnetization ($\mathbf{M}(\mathbf{r}, t)$), and the quantities $\partial \mathbf{P}(\mathbf{r}, t) / \partial t$ and $\nabla \times \mathbf{M}(\mathbf{r}, t)$ are named the polarization and magnetization current densities, respectively. In macroscopic (macro) electrodynamics, one first defines $\mathbf{P}^{\text{macro}}$ and $\mathbf{M}^{\text{macro}}$ as the electric and magnetic dipole moments of all the particles in a small volume divided by the magnitude of this volume, taken in the limit where the volume shrinks to a macroscopically small size, a size which however still must be large on the microscopic length scale [19, 43]. The macroscopic current densities $\partial \mathbf{P}^{\text{macro}}(\mathbf{r}, t) / \partial t$ and $\nabla \times \mathbf{M}^{\text{macro}}(\mathbf{r}, t)$ then are introduced, and their sum is $\mathbf{J}^{\text{macro}}(\mathbf{r}, t)$. In the microscopic (classical) description, one in a sense proceeds in the opposite way. The current density field, $\mathbf{J}(\mathbf{r}, t)$, is a well-defined quantity, and the definition in (10.41) introduces, with some arbitrariness as we shall realize, generalized polarization and magnetization concepts. By a division of $\mathbf{J}$, $\mathbf{P}$, and $\mathbf{M}$ into

their transverse ($\mathbf{J}_T$, $\mathbf{P}_T$, $\mathbf{M}_T$) and longitudinal ($\mathbf{J}_L$, $\mathbf{P}_L$, $\mathbf{M}_L$) parts, one obtains

$$\mathbf{J}_L(\mathbf{r}, t) = \frac{\partial}{\partial t} \mathbf{P}_L(\mathbf{r}, t), \quad (10.42)$$

and

$$\mathbf{J}_T(\mathbf{r}, t) = \frac{\partial}{\partial t} \mathbf{P}_T(\mathbf{r}, t) + \nabla \times \mathbf{M}_T(\mathbf{r}, t). \quad (10.43)$$

It is obvious from (10.41) (and (10.42)) that the longitudinal part $\mathbf{M}_L(\mathbf{r}, t)$ of the magnetization vector field does not play any physical role since only $\nabla \times \mathbf{M}(\mathbf{r}, t) = \nabla \times \mathbf{M}_T(\mathbf{r}, t)$ contributes to the microscopic current density. Despite of this fact, it is in certain situations useful to introduce a specific $\mathbf{M}_L$ -vector field. Whatever choice is made for $\mathbf{M}_L(\mathbf{r}, t)$ in a given calculation the final (physical) result will never depend on $\mathbf{M}_L(\mathbf{r}, t)$. By taking the divergence of (10.42), a comparison to the equation of continuity, $\nabla \cdot \mathbf{J} = -\partial \rho / \partial t$, leads to

$$\rho(\mathbf{r}, t) = -\nabla \cdot \mathbf{P}_L(\mathbf{r}, t). \quad (10.44)$$

Since $\nabla \times \mathbf{P}_L = \mathbf{0}$, Helmholtz theorem shows that the longitudinal part of the generalized polarizability is completely fixed by the charge density $\rho(\mathbf{r}, t)$. The transverse parts of the generalized polarizability and magnetization are not given uniquely by the division in (10.43). Thus, if $\mathbf{N}_T(\mathbf{r}, t)$ is an arbitrary transverse vector field, yet differentiable in space and time, the transformation

$$\mathbf{P}_T(\mathbf{r}, t) \Rightarrow \mathbf{P}'_T(\mathbf{r}, t) = \mathbf{P}_T(\mathbf{r}, t) - \nabla \times \mathbf{N}_T(\mathbf{r}, t), \quad (10.45)$$

$$\mathbf{M}_T(\mathbf{r}, t) \Rightarrow \mathbf{M}'_T(\mathbf{r}, t) = \mathbf{M}_T(\mathbf{r}, t) + \frac{\partial}{\partial t} \mathbf{N}_T(\mathbf{r}, t), \quad (10.46)$$

does not alter the transverse part of the microscopic current density, i.e., $\mathbf{J}'_T(\mathbf{r}, t) = \mathbf{J}_T(\mathbf{r}, t)$. Different choices can hence be made for the differentiable vector fields $\mathbf{P}_T$ and $\mathbf{M}_T$, the only restriction being the requirement that the divergence-free part of the microscopic current density in (10.43) must be an invariant quantity. The choice $\partial \mathbf{N}_T / \partial t = -\mathbf{M}_T$ eliminates the generalized magnetization $\mathbf{M}_T$ completely, and allows one to formulate the general (linear) response theory solely on the basis of a microscopic polarization, i.e., via $\mathbf{J} = \partial \mathbf{P}_L / \partial t + \partial \mathbf{P}'_T / \partial t$. Since $\mathbf{P}_L$ is fixed it is not possible to eliminate $\mathbf{P}$ completely in favor of $\mathbf{M} = \mathbf{M}_T$. The transverse part of $\mathbf{P}$ can be eliminated with the choice $\nabla \times \mathbf{N}_T = \mathbf{P}_T$, and if this choice is made one has $\mathbf{J} = \partial \mathbf{P}_L / \partial t + \nabla \times \mathbf{M}'_T$, where $\mathbf{M}'_T = \mathbf{M}_T + \partial \mathbf{N}_T / \partial t$. The $\mathbf{N}_T$ -vector field appearing here is of course completely specied because $\nabla \times \mathbf{N}_T = \mathbf{P}_T$ and $\nabla \cdot \mathbf{N}_T = 0$.

10.4.2 Generalized Electric Displacement and Magnetic Vector Fields

Let us assume that we have made a certain choice for $\mathbf{P}_T$ and $\mathbf{M}_T$. For this choice we *define* a generalized electric displacement field $\mathbf{D}(\mathbf{r}, t)$ via

$$\mathbf{D}(\mathbf{r}, t) = \epsilon_0 \mathbf{E}(\mathbf{r}, t) + \mathbf{P}(\mathbf{r}, t), \quad (10.47)$$

and a new magnetic vector field $\mathbf{H}(\mathbf{r}, t)$ by the relation

$$\mathbf{H}(\mathbf{r}, t) = \mu_0^{-1} \mathbf{B}(\mathbf{r}, t) - \mathbf{M}(\mathbf{r}, t). \quad (10.48)$$

The new fields are microscopic quantities, which in the macroscopic limit become identical to those introduced in macroscopic electrodynamics.

The longitudinal part of the $\mathbf{D}$ -field, given by

$$\mathbf{D}_L(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_L(\mathbf{r}, t) + \mathbf{P}_L(\mathbf{r}, t), \quad (10.49)$$

is independent of the specific choice made, and furthermore independent of the dynamics in the system we excite by the external electromagnetic field. To prove the last claim we combine the Maxwell equation $\nabla \cdot \mathbf{E}_L(\mathbf{r}, t) = (\rho + \rho^{\text{ext}})/\epsilon_0$ with (10.44) and (10.49) and obtain readily

$$\nabla \cdot \mathbf{D}_L(\mathbf{r}, t) = \rho^{\text{ext}}(\mathbf{r}, t). \quad (10.50)$$

The longitudinal part of the electric displacement field hence is determined completely by the prescribed external charge density. Since $\rho^{\text{ext}}(\mathbf{r}, t)$ is a microscopic quantity, it is related to the longitudinal part of the microscopic *external* electric field by the Maxwell–Lorentz equation

$$\nabla \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}, t) = \epsilon_0^{-1} \rho^{\text{ext}}(\mathbf{r}, t). \quad (10.51)$$

Together, (10.50) and (10.51) lead to the conclusion

$$\mathbf{D}_L(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_L^{\text{ext}}(\mathbf{r}, t). \quad (10.52)$$

The transverse part of the dielectric displacement field, viz.,

$$\mathbf{D}_T(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_T(\mathbf{r}, t) + \mathbf{P}_T(\mathbf{r}, t) \quad (10.53)$$

of course depends on the choice made for $\mathbf{P}_T$, cf. (10.45).

The magnetic $\mathbf{B}$ -field is a transverse vector field, and the longitudinal part of the $\mathbf{H}$ -field defined in (10.48) therefore is given by $\mathbf{H}_L(\mathbf{r}, t) = -\mathbf{M}_L(\mathbf{r}, t)$, but since $\mathbf{M}_L(\mathbf{r}, t)$ is of no physical significance, $\mathbf{H}_L(\mathbf{r}, t)$ plays no physical role either. The

transverse part of the magnetic $\mathbf{H}$ -field, namely,

$$\mathbf{H}_T(\mathbf{r}, t) = \mu_0^{-1} \mathbf{B}_T(\mathbf{r}, t) - \mathbf{M}_T(\mathbf{r}, t) \quad (10.54)$$

depends on the choice made for the transverse part of the magnetization.

10.4.3 Central Field Equations

The introduction of the $\mathbf{D}$ - and $\mathbf{H}$ -fields, via the definitions in (10.47) and (10.48), implies that the inhomogeneous Maxwell–Lorentz equations in (2.2) and (2.3) can be written in a somewhat different form, as we shall realize now. The charge and current densities appearing in these equations include *all* particles, and to comply with the notation of Sect. 10.4.1 one must make the replacements $\mathbf{J} \Rightarrow \mathbf{J}^{\text{tot}} = \mathbf{J}^{\text{ext}} + \mathbf{J}$, and $\rho \Rightarrow \rho^{\text{total}} = \rho^{\text{ext}} + \rho$ in (2.2) and (2.3). Subsequently, substitution of the expression for $\mathbf{J}$ given in (10.41) replaces (2.2) by the equation

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \mu_0 \frac{\partial \mathbf{P}(\mathbf{r}, t)}{\partial t} + \mu_0 \nabla \times \mathbf{M}(\mathbf{r}, t) + \mu_0 \mathbf{J}^{\text{ext}}(\mathbf{r}, t) + c_0^{-2} \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t}, \quad (10.55)$$

and use of (10.47) and (10.48) finally brings the Maxwell–Lorentz equation in (2.3) into the form

$$\nabla \times \mathbf{H}(\mathbf{r}, t) = \mathbf{J}^{\text{ext}}(\mathbf{r}, t) + \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t}. \quad (10.56)$$

Although this equation in notation resembles a well-known macroscopic Maxwell equation, it *is* a microscopic field equation. The longitudinal part of the equation, namely,

$$\mathbf{J}_L^{\text{ext}}(\mathbf{r}, t) + \frac{\partial}{\partial t} \mathbf{D}_L(\mathbf{r}, t) = \mathbf{0}, \quad (10.57)$$

relates $\mathbf{D}_L$ solely to the external dynamics (via $\mathbf{J}_L^{\text{ext}}$). This was to be expected on the basis of (10.50). From (10.50) and (10.57) follow the equation of continuity for the external particle distribution, i.e., $\nabla \cdot \mathbf{J}_L^{\text{ext}} + \partial \rho^{\text{ext}} / \partial t = 0$. The transverse part

$$\nabla \times \mathbf{H}_T(\mathbf{r}, t) - \frac{\partial}{\partial t} \mathbf{D}_T(\mathbf{r}, t) = \mathbf{J}_T^{\text{ext}}(\mathbf{r}, t), \quad (10.58)$$

of (10.56), and the transverse homogeneous Maxwell equation

$$\nabla \times \mathbf{E}_T(\mathbf{r}, t) + \frac{\partial}{\partial t} \mathbf{B}_T(\mathbf{r}, t) = \mathbf{0}, \quad (10.59)$$

are the central field equations for the response theory to be described in Sect. 10.5. Although the fields $\mathbf{H}_T$ and $\mathbf{D}_T$ depend on the choice made for $\mathbf{M}_T$ and $\mathbf{P}_T$, one easily shows by an explicit calculation that the left side of (10.58) is the same for all choices, as it must be because $\mathbf{J}_T^{\text{ext}}$ is a fixed microscopic quantity. Together, (2.1),

(2.4), (10.50) (and possibly with $\mathbf{D}_L$ replaced by $\mathbf{D}$), and (10.56) appear in a form completely identical to that of the well-known macroscopic Maxwell equations, but the reader should remember that our new equations in fact are rigorous microscopic field equations.

10.5 Response Theory Based on Generalized Permittivity and Permeability Tensors for Transverse Dynamics

10.5.1 Flexibility

In the framework of linear response theory, the transverse set of Maxwell–Lorentz equations in (9.25) and (9.26) is closed by introduction of the constitutive equation in (10.2). In nonrelativistic electrodynamics, the microscopic response tensor $\boldsymbol{\Sigma}_T(\mathbf{r}, \mathbf{r}', t, t')$ in principle can be determined via the many-body Schrödinger equation for the system under study. A certain flexibility in the formulation of the linear response theory can be obtained by replacing $\boldsymbol{\Sigma}_T$ with *two* new interrelated response tensors. The introduction of these tensors is closely related to the division in (10.43) of the transverse current density into parts related to the generalized polarization and magnetization. The transverse part of the dielectric displacement we thus relate to the transverse local electric field via a spatially and timely nonlocal constitutive relation

$$\mathbf{D}_T(\mathbf{r}, t) = \epsilon_0 \int_{-\infty}^{\infty} \boldsymbol{\epsilon}_T(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3 r', \quad (10.60)$$

where $\boldsymbol{\epsilon}_T(\mathbf{r}, \mathbf{r}', t, t')$ is the so-called generalized relative permittivity (dielectric) tensor belonging to the transverse (subscript T) dynamics. The other new response tensor relates the microscopic $\mathbf{B}$ and $\mathbf{H}_T^{\text{ext}}$ fields as follows:

$$\mathbf{B}(\mathbf{r}, t) = \mu_0 \int_{-\infty}^{\infty} \boldsymbol{\mu}_T(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{H}_T^{\text{ext}}(\mathbf{r}', t') dt' d^3 r'. \quad (10.61)$$

The quantity $\boldsymbol{\mu}_T(\mathbf{r}, \mathbf{r}', t, t')$ is called the generalized relative (magnetic) permeability tensor. Although, only transverse dynamics enters the physics of the “magnetic” response ($\mathbf{B} = \mathbf{B}_T$ always; $\mathbf{H}_L$ of no physical significance) it is convenient to add a subscript T to $\boldsymbol{\mu}$. In the following I shall, as it is often done, leave out the word “relative” when referring to $\boldsymbol{\epsilon}_T$ and $\boldsymbol{\mu}_T$. The arbitrariness in the generalized polarization and magnetization fields, as expressed in (10.45) and (10.46) is transferred to $\boldsymbol{\epsilon}_T$ and $\boldsymbol{\mu}_T$ via (10.53) and (10.54). The fact that $\boldsymbol{\epsilon}_T$ and $\boldsymbol{\mu}_T$ have no unique physical meaning allows one to make different interrelated choices for these tensors without affecting any physical conclusions arising from calculations based on a given choice. In a given application one choice may be better than others from a calculational point of view.

10.5.2 Response Theory Based on the Choice

$$\mu_{\text{T}}(\mathbf{r}, \mathbf{r}', t, t') = U\delta(\mathbf{r} - \mathbf{r}')\delta(t - t')$$

We have realized in Sect. 10.4.1 that it is possible to make the choice $\mathbf{M}_{\text{T}} = \mathbf{0}$. With this choice all “magnetic” effects are described via the transverse part of the microscopic polarization field, $\mathbf{P}_{\text{T}}$. For $\mathbf{M}_{\text{T}} = \mathbf{0}$ one gets from (10.54) $\mathbf{B}_{\text{T}}(\mathbf{r}, t) = \mu_0 \mathbf{H}_{\text{T}}(\mathbf{r}, t)$, and consequently

$$\mu_{\text{T}}(\mathbf{r}, \mathbf{r}', t, t') = U\delta(\mathbf{r} - \mathbf{r}')\delta(t - t'), \quad (10.62)$$

as is readily seen by combination of (10.61) and (10.62). The generalized permittivity which is related to this choice for μ_{T} I denote by $\epsilon_{\text{T}}^{\text{PM}}$, and the superscript PM is used to remind us that both “polarization (P)” and “magnetization (M)” effects are included in this response tensor. Thus,

$$\mathbf{D}_{\text{T}}(\mathbf{r}, t) = \epsilon_0 \int_{-\infty}^{\infty} \epsilon_{\text{T}}^{\text{PM}}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_{\text{T}}^{\text{ext}}(\mathbf{r}', t') dt' d^3 r' \quad (10.63)$$

and since $\mathbf{M}_{\text{T}} = \mathbf{0}$, the transverse current density is given by

$$\mathbf{J}_{\text{T}}(\mathbf{r}, t) = \frac{\partial}{\partial t} \mathbf{P}_{\text{T}}(\mathbf{r}, t). \quad (10.64)$$

To determine the relation between the transverse conductivity tensor $\Sigma_{\text{T}}(\mathbf{r}, \mathbf{r}', t, t')$ (10.3) and $\epsilon_{\text{T}}^{\text{PM}}(\mathbf{r}, \mathbf{r}', t, t')$ one differentiates (10.53) with respect to time and makes use of (10.64). Hence,

$$\frac{\partial}{\partial t} \mathbf{D}_{\text{T}}(\mathbf{r}, t) = \epsilon_0 \frac{\partial}{\partial t} \mathbf{E}_{\text{T}}(\mathbf{r}, t) + \mathbf{J}_{\text{T}}(\mathbf{r}, t). \quad (10.65)$$

By insertion of the constitutive equations in (10.2) and (10.63) into (10.65) one obtains the connection

$$\Sigma_{\text{T}}(\mathbf{r}, \mathbf{r}', t, t') = \epsilon_0 \frac{\partial}{\partial t} (\epsilon_{\text{T}}^{\text{PM}}(\mathbf{r}, \mathbf{r}', t, t') - U\delta(\mathbf{r} - \mathbf{r}')\delta(t - t')). \quad (10.66)$$

For systems translationally invariant in time one has the relation

$$\epsilon_{\text{T}}^{\text{PM}}(\mathbf{r}, \mathbf{r}'; \omega) = U\delta(\mathbf{r} - \mathbf{r}') + \frac{i}{\epsilon_0 \omega} \Sigma_{\text{T}}(\mathbf{r}, \mathbf{r}'; \omega). \quad (10.67)$$

in the space–frequency domain.

10.5.3 Response Theory Based on the Choice

$$\mathbf{D}_T(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$$

We have realized in Sect. 10.4.2 that the longitudinal part of the electric displacement divided by ϵ_0 is just the longitudinal part of the external electric field, i.e., $\mathbf{D}_L(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_L^{\text{ext}}(\mathbf{r}, t)$ (10.52). Combined with the choice $\mathbf{D}_T(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$ one, therefore, gets $\mathbf{D}(\mathbf{r}, t) = \epsilon_0 \mathbf{E}^{\text{ext}}(\mathbf{r}, t)$. For reasons soon to become clear, the constitutive relation giving the connection between $\mathbf{D}_T = \epsilon_0 \mathbf{E}_T^{\text{ext}}$ and $\mathbf{E}_T$ after division with ϵ is written as follows:

$$\mathbf{E}_T^{\text{ext}}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{L}_T^{-1}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') dt' d^3 r'. \quad (10.68)$$

The kernel in (10.68) is denoted by $\mathbf{L}_T^{-1}(\mathbf{r}, \mathbf{r}', t, t')$ because it in a generalized sense is the reciprocal of the causal transverse local-field tensor $\mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t')$ relating $\mathbf{E}_T$ and $\mathbf{E}_T^{\text{ext}}$ in the manner given in (10.7). Thus, if the integral relation

$$\int_{-\infty}^{\infty} \mathbf{L}_T(\mathbf{r}, \mathbf{r}'', t, t'') \cdot \mathbf{L}_T^{-1}(\mathbf{r}'', \mathbf{r}', t'', t') dt'' d^3 r'' = \mathbf{U} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \quad (10.69)$$

holds between $\mathbf{L}_T$ and $\mathbf{L}_T^{-1}$, the solution of the integral equation in (10.68) with respect to the local field $\mathbf{E}_T$ is precisely the one given in (10.7). The reader may convince herself of this by insertion of (10.68) into (10.7), and afterwards use of (10.69). The generalized permittivity tensor related to the choice $\mathbf{D}_T(\mathbf{r}, t) = \epsilon_0 \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$, hence, is the “inverse,” $\mathbf{L}_T^{-1}(\mathbf{r}, \mathbf{r}', t, t')$, of the transverse local-field tensor $\mathbf{L}_T(\mathbf{r}, \mathbf{r}', t, t')$.

With the above-mentioned choice one also obtains $\mathbf{H}_T(\mathbf{r}, t) = \mu_0^{-1} \mathbf{B}^{\text{ext}}(\mathbf{r}, t)$. To prove this, let us insert the relation $\mathbf{D}_T = \epsilon_0 \mathbf{E}_T^{\text{ext}}$ into the central equation in (10.58). Thus,

$$\nabla \times \mathbf{H}_T(\mathbf{r}, t) = \mathbf{J}_T^{\text{ext}}(\mathbf{r}, t) + \epsilon_0 \frac{\partial}{\partial t} \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t). \quad (10.70)$$

The external charge distribution is the source of the external fields $\mathbf{E}^{\text{ext}}(\mathbf{r}, t)$ and $\mathbf{B}^{\text{ext}}(\mathbf{r}, t)$, and the following Maxwell–Lorentz equation must therefore hold for the transverse dynamics:

$$\nabla \times \mathbf{B}^{\text{ext}}(\mathbf{r}, t) = \mu_0 \mathbf{J}_T^{\text{ext}}(\mathbf{r}, t) + c_0^{-2} \frac{\partial}{\partial t} \mathbf{E}_T^{\text{ext}}(\mathbf{r}, t). \quad (10.71)$$

A comparison of (10.70) and (10.71) immediately leads to the claimed result $\mathbf{H}_T(\mathbf{r}, t) = \mu_0^{-1} \mathbf{B}^{\text{ext}}(\mathbf{r}, t)$. The constitutive relation in (10.61) in turn takes the form

$$\mathbf{B}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \boldsymbol{\mu}_T^{\text{CAU}}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{B}^{\text{ext}}(\mathbf{r}', t') dt' d^3 r'. \quad (10.72)$$

The generalized permeability tensor denoted by $\mu_T^{\text{CAU}}(\mathbf{r}, \mathbf{r}', t, t')$, hence relates the local and external $\mathbf{B}$ -fields. In the framework of response theory, the related response tensor is causal, and this has been emphasized by the superscript CAU.

10.6 Response to External Longitudinal Fields

In near-field electrodynamics, the source and object to be investigated often are placed so close to each other that (some of) the object particles are within the rim zone of the external field. In such cases, not only the transverse part of the external electromagnetic field but also the longitudinal external electric field, $\mathbf{E}_L^{\text{ext}}$, give rise to induced microscopic currents in the object under study. These currents in turn create electromagnetic fields which may act back and affect the source particle dynamics. The importance of the back-action most often increases when the source and object are brought closer to each other. If the back-action is appreciable response theory can no longer be applied and the source and object have to be treated electrostatically as one system.

Let us assume that the back-action is negligible and that the externally impressed longitudinal electric field is so weak that linear response theory can be used. A constitutive relation of the form

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{R}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t') dt' d^3 r' \quad (10.73)$$

then links the prescribed longitudinal external electric field to the current density $\mathbf{J}(\mathbf{r}, t)$ induced by this field. As indicated, the constitutive relation will in general be nonlocated in both space and time. It is obvious that the relation in (10.73) is causal, and the response tensor $\mathbf{R}(\mathbf{r}, \mathbf{r}', t, t')$ therefore satisfies the condition

$$\mathbf{R}(\mathbf{r}, \mathbf{r}', t, t'(> t)) = \mathbf{0}. \quad (10.74)$$

The transverse and longitudinal parts of the current density in (10.73) can be obtained in the usual manner by means of (9.17) and (9.18). Hence,

$$\mathbf{J}_I(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{R}_I(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t') dt' d^3 r', \quad (10.75)$$

where

$$\mathbf{R}_I(\mathbf{r}, \mathbf{r}', t, t') = \int_{-\infty}^{\infty} \delta_I(\mathbf{r} - \mathbf{r}'') \cdot \mathbf{R}(\mathbf{r}'', \mathbf{r}', t, t') d^3 r''. \quad (10.76)$$

for $I = T$ and L .

10.7 The General Constitutive Relation

By now we have at hand two pieces which allow us to establish the linear constitutive relation in its most general form. The current density distribution induced in the medium under study thus is the sum of the distributions induced by say the self-consistent transverse field and the longitudinal part of the source field, and these distributions can be obtained from (10.1) and (10.73). Hence,

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} [\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') + \mathbf{R}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t')] dt' d^3 r'. \quad (10.77)$$

Formally, one may replace (10.1) by (10.10) and thus present the general constitutive relation in the form

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} [\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}', t') + \mathbf{R}(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t')] dt' d^3 r'. \quad (10.78)$$

Although both response tensors appearing in (10.78) are causal, (10.78) is in general not so convenient: Response tensors $\boldsymbol{\Sigma}$ and $\mathbf{R}$ in principle can be determined alone from the relevant quantum mechanical wave equation (Shrödinger, Pauli, or Dirac equation) whereas the determination of $\boldsymbol{\sigma}$ also requires a calculation of the transverse local-field tensor $\mathbf{L}_T$, cf. the analysis in Sects. 10.1.2 and 10.1.3. The following two chapters are devoted to the nonrelativistic quantum mechanical calculation of $\boldsymbol{\Sigma}$ and $\mathbf{R}$. The constitutive relation in (10.77) can be written in compact form as follows:

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{r}, \mathbf{r}', t, t') \cdot (\mathbf{E}_T(\mathbf{r}', t') + \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t')) dt' d^3 r', \quad (10.79)$$

and the four “dyadic delta function projections”

$$\mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}', t, t') = \int_{-\infty}^{\infty} \delta_A(\mathbf{r} - \mathbf{r}'') \cdot \mathbf{S}(\mathbf{r}'', \mathbf{r}''', t, t') \cdot \delta_B(\mathbf{r}''' - \mathbf{r}') d^3 r'' d^3 r''', \quad (10.80)$$

where A, B = T or L, give us the response tensors $\boldsymbol{\Sigma}$ and $\mathbf{R}$. Thus, $\boldsymbol{\Sigma} = \mathbf{S}_{TT} + \mathbf{S}_{LT}$ and $\mathbf{R} = \mathbf{S}_{TL} + \mathbf{S}_{LL}$.

Inside the rim zone of the system the *induced* longitudinal current density, $\mathbf{J}_L(\mathbf{r}, t)$, and the *induced* longitudinal electric field, given by $\mathbf{E}_L(\mathbf{r}, t) - \mathbf{E}_L^{\text{ext}}(\mathbf{r}, t)$ (since $\mathbf{E}_L(\mathbf{r}, t)$ denotes the *total* field), are related via the longitudinal part of the Maxwell–Lorentz equations. Thus, from (9.27) (where $\mathbf{J}_L$ and $\mathbf{E}_L$ are the *total* fields) one obtains

$$\mathbf{J}_L(\mathbf{r}, t) = -\epsilon_0 \frac{\partial}{\partial t} (\mathbf{E}_L(\mathbf{r}, t) - \mathbf{E}_L^{\text{ext}}(\mathbf{r}, t)). \quad (10.81)$$

Then, in the framework of the microscopic classical electrodynamics, and by means of (9.54), the quite complicated relation

$$\begin{aligned} & \int_{-\infty}^{\infty} [\boldsymbol{\Sigma}_L(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_T(\mathbf{r}', t') + \mathbf{R}_L(\mathbf{r}, \mathbf{r}', t, t') \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}', t')] dt' d^3 r' \\ &= -\frac{1}{4\pi} \frac{\partial}{\partial t} \left[\sum_{\alpha} q_{\alpha} \frac{\mathbf{r} - \mathbf{r}_{\alpha}(t)}{|\mathbf{r} - \mathbf{r}_{\alpha}(t)|^3} \right] \end{aligned} \quad (10.82)$$

follows. The index α runs over all the particles of the system, and $\boldsymbol{\Sigma}_L = \boldsymbol{\Sigma} - \boldsymbol{\Sigma}_T$.

10.8 Response Tensors for Media with Finite and Infinitesimal Translational Invariance in Space

10.8.1 Lattice Periodicity

In studies of the microscopic electrodynamic bulk properties of crystalline solids, it is usually a good approximation to assume that the relevant microscopic response tensors are invariant against lattice-vector displacements. The approximation leads to a substantial simplification of the linear response theory in the wave-vector domain, as we shall realize now. To be specific, we carry out the analysis for the generalized response tensor $\mathbf{S}$ entering the constitutive relation in (10.79), but analogous analyzes can be done for the other response tensors introduced in this chapter. Without loss of essential generality we limit ourselves to media exhibiting translational invariance in time, so that $\mathbf{S}(\mathbf{r}, \mathbf{r}', t, t') = \mathbf{S}(\mathbf{r}, \mathbf{r}', t - t')$. The assumption of translational invariance of the electrodynamic properties of the medium against lattice-vector displacements implies that the space–frequency representative of $\mathbf{S}$ satisfies the condition

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = \mathbf{S}(\mathbf{r} + \mathbf{R}_L, \mathbf{r}' + \mathbf{R}_L; \omega) \quad (10.83)$$

for the arbitrary lattice (L) vector $\mathbf{R}_L$. The Fourier integral representation

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = (2\pi)^{-6} \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{q}, \mathbf{q}', \omega) e^{i\mathbf{q} \cdot \mathbf{r}} e^{i\mathbf{q}' \cdot \mathbf{r}'} d^3 q' d^3 q \quad (10.84)$$

and (10.83) together imply that the Fourier amplitude must fulfil the condition

$$\mathbf{S}(\mathbf{q}, \mathbf{q}', \omega) = \mathbf{S}(\mathbf{q}, \mathbf{q}', \omega) e^{i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{R}_L}. \quad (10.85)$$

Therefore, the wave vectors $\mathbf{q}$ and $\mathbf{q}'$ are not independent but related via the equation

$$\mathbf{q} + \mathbf{q}' = \mathbf{G}, \quad (10.86)$$

where $\mathbf{G}$ is a reciprocal lattice vector. The condition in (10.85) shows that one may write the wave-vector representative of the response tensor in the form

$$\mathbf{S}(\mathbf{q}, \mathbf{q}', \omega) = (2\pi)^3 \sum_{\mathbf{G}} \mathbf{S}(\mathbf{q}, \mathbf{G} - \mathbf{q}, \omega) \delta(\mathbf{q} + \mathbf{q}' - \mathbf{G}), \quad (10.87)$$

where the summation runs over all reciprocal lattice vectors.

The result in (10.87) has the consequence that the constitutive relation in (10.79) (for $\mathbf{S}(\mathbf{r}, \mathbf{r}', t, t') = \mathbf{S}(\mathbf{r}, \mathbf{r}', t - t')$) takes an algebraic form in the wave vector–frequency domain. By insertion of spatial Fourier integrals for $\mathbf{J}(\mathbf{r}; \omega)$, $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ (two integrals), and $\mathbf{E}_T(\mathbf{r}; \omega) + \mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega)$ into the space–frequency representative of (10.79), and afterwards use of the plane-wave expansion of the Dirac delta function, the reader may verify that

$$\mathbf{J}(\mathbf{q}, \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{q}, \mathbf{q}', \omega) \cdot [\mathbf{E}_T(-\mathbf{q}', \omega) + \mathbf{E}_L^{\text{ext}}(-\mathbf{q}', \omega)] d^3 q'. \quad (10.88)$$

With $\mathbf{S}(\mathbf{q}, \mathbf{q}', \omega)$ given by (10.87) the integration over $\mathbf{q}'$ in (10.88) is readily carried out, and the expression for the current density finally reduces to the following sum of terms:

$$\mathbf{J}(\mathbf{q}, \omega) = \sum_{\mathbf{G}} \mathbf{S}(\mathbf{q}, \mathbf{G} - \mathbf{q}, \omega) \cdot [\mathbf{E}_T(\mathbf{q} - \mathbf{G}, \omega) + \mathbf{E}_L^{\text{ext}}(\mathbf{q} - \mathbf{G}, \omega)]. \quad (10.89)$$

10.8.2 Slowly Varying External Fields

Calculations analogous to those presented in Sect. 10.8.1 of course lead to the conclusion that the constitutive equation in (10.78) for lattice-periodic media exhibiting translational invariance in time can be reduced to the form

$$\begin{aligned} \mathbf{J}(\mathbf{q}, \omega) = \sum_{\mathbf{G}} & [\boldsymbol{\sigma}(\mathbf{q}, \mathbf{G} - \mathbf{q}, \omega) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{q} - \mathbf{G}, \omega) \\ & + \mathbf{R}(\mathbf{q}, \mathbf{G} - \mathbf{q}, \omega) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{q} - \mathbf{G}, \omega)] \end{aligned} \quad (10.90)$$

in the $(\omega, \mathbf{q})$ -domain. In near-field optics, and in physical optics as such, one usually can assume with extremely high accuracy that the transverse part of the external electromagnetic field does not vary on the atomic length scale. The wave-vector spectrum of $\mathbf{E}_T^{\text{ext}}$, hence, only contains wave vectors $\mathbf{q}^{\text{ext}}$ satisfying $|\mathbf{q}^{\text{ext}}| \ll |\mathbf{G}|$ for all $\mathbf{G}$. Although the longitudinal part of the external field may vary quite rapidly in space across a mesoscopic object (or structure) when this is placed in the rim zone of the source, the approximation $|\mathbf{q}^{\text{ext}}| \ll |\mathbf{G}|$ usually is also satisfied for the wave-vector spectrum of $\mathbf{E}_L^{\text{ext}}$. According to (10.90) an external electric field of wave vector $\mathbf{q}^{\text{ext}}$ in general generates currents not only at $\mathbf{q}^{\text{ext}}$ but at all wave vectors

displaced from $\mathbf{q}^{\text{ext}}$ by a reciprocal lattice vector $\mathbf{G}$. In the optical regime (and at frequencies below), the current densities at $\mathbf{J}(\mathbf{q}^{\text{ext}} + \mathbf{G}, \omega)$ [$\mathbf{G} \neq \mathbf{0}$] are usually small, and if they are completely neglected one obtains

$$\begin{aligned} \mathbf{J}(\mathbf{q}^{\text{ext}}, \omega) = & \boldsymbol{\sigma}(\mathbf{q}^{\text{ext}}, -\mathbf{q}^{\text{ext}}, \omega) \cdot \mathbf{E}_{\text{T}}^{\text{ext}}(\mathbf{q}^{\text{ext}}, \omega) \\ & + \mathbf{R}(\mathbf{q}^{\text{ext}}, -\mathbf{q}^{\text{ext}}, \omega) \cdot \mathbf{E}_{\text{L}}^{\text{ext}}(\mathbf{q}^{\text{ext}}, \omega). \end{aligned} \quad (10.91)$$

In direct space, the response function $\boldsymbol{\sigma}$ is calculated from

$$\boldsymbol{\sigma}(\mathbf{r} - \mathbf{r}'; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \boldsymbol{\sigma}(\mathbf{q}, -\mathbf{q}, \omega) \delta(\mathbf{q} + \mathbf{q}') e^{i\mathbf{q} \cdot \mathbf{r}} e^{i\mathbf{q}' \cdot \mathbf{r}'} d^3q d^3q' \quad (10.92)$$

in this limit, cf. (10.84) and (10.87). As already indicated on the left side of (10.92) the response tensor now only depends on the difference $\mathbf{r} - \mathbf{r}'$, i.e., $\boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}'; \omega) = \boldsymbol{\sigma}(\mathbf{r} - \mathbf{r}'; \omega)$. For the response tensor $\mathbf{R}$ we of course also obtain the result $\mathbf{R}(\mathbf{r}, \mathbf{r}'; \omega) = \mathbf{R}(\mathbf{r} - \mathbf{r}'; \omega)$ when (10.91) holds. For external fields sufficiently slowly varying in space a crystalline medium usually appears to possess infinitesimal translational invariance. With the abbreviations $\boldsymbol{\sigma}(\mathbf{q}, -\mathbf{q}, \omega) \equiv \boldsymbol{\sigma}(\mathbf{q}, \omega)$ and $\mathbf{R}(\mathbf{q}, -\mathbf{q}, \omega) = \mathbf{R}(\mathbf{q}, \omega)$ we thus have

$$\mathbf{J}(\mathbf{q}, \omega) = \boldsymbol{\sigma}(\mathbf{q}, \omega) \cdot \mathbf{E}_{\text{T}}^{\text{ext}}(\mathbf{q}, \omega) + \mathbf{R}(\mathbf{q}, \omega) \cdot \mathbf{E}_{\text{L}}^{\text{ext}}(\mathbf{q}, \omega) \quad (10.93)$$

for media which effectively exhibit infinitesimal translational invariance in time and space. If one further can assume that the medium effectively appears isotropic, $\mathbf{E}_{\text{T}}^{\text{ext}}$ generates only transverse current densities, $\mathbf{J}_{\text{T}}(\mathbf{q}, \omega) = (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{J}(\mathbf{q}, \omega)$, and $\mathbf{E}_{\text{L}}^{\text{ext}}$ only longitudinal current densities $\mathbf{J}_{\text{L}}(\mathbf{q}, \omega) = \hat{\mathbf{q}}\hat{\mathbf{q}} \cdot \mathbf{J}(\mathbf{q}, \omega)$. The related response tensors often are named the transverse ($\boldsymbol{\sigma}(\mathbf{q}, \omega)$) and longitudinal ($\mathbf{R}(\mathbf{q}, \omega)$) microscopic conductivity. The isotropic response tensors are very useful quantities in studies of the microscopic (near-field) optical properties of metals (in the solid-state plasma or jellium approximation [195]) and BCS superconductors [98].

When quantum wells, surfaces and interfaces are studied by near-field optical methods, e.g., with evanescent waves, lattice periodicity can often be assumed in the plane of the well or parallel to the surface (interface). For such studies, the response tensor in (10.87), must be replaced by a mixed response tensor of the form

$$\mathbf{S}(z, z'; \mathbf{q}_{\parallel}, \mathbf{q}'_{\parallel}, \omega) = (2\pi)^2 \sum_{\mathbf{G}_{\parallel}} \mathbf{S}(z, z', \mathbf{q}_{\parallel}, \mathbf{G}_{\parallel} - \mathbf{q}_{\parallel}, \omega) \delta(\mathbf{q}_{\parallel} + \mathbf{q}'_{\parallel} - \mathbf{G}_{\parallel}), \quad (10.94)$$

where $\mathbf{G}_{\parallel}$ is a 2D reciprocal lattice vector in the plane of the well (surface, interface), and $z(z')$ is the Cartesian coordinate perpendicular to this plane. The analysis of the 2D response can be carried out along the same lines as done for the 3D response above.

Chapter 11

Density Matrix Formalism: Hamilton and Current Density Operators – Gauge Invariance

In Chap. 10, we discussed the microscopic linear response theory from a general point of view paying special attention to spatial nonlocality. The response tensors $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ and $\mathbf{R}(\mathbf{r}, \mathbf{r}'; \omega)$, describing the microscopic current density ($\mathbf{J}(\mathbf{r}; \omega)$) induced by the transverse part ($\mathbf{E}_T(\mathbf{r}; \omega)$) of the local electric field and the longitudinal part ($\mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega)$) of the external field, respectively, played a central role in our discussion but no attempts were made to carry out an explicit calculation of these quantities. In Chap. 12, we shall on the basis of the Liouville equation for the density matrix operator carry out a nonrelativistic quantum physical calculation of $\boldsymbol{\Sigma}(\mathbf{r}, \mathbf{r}'; \omega)$ and $\mathbf{R}(\mathbf{r}, \mathbf{r}'; \omega)$. As a forerunner for this calculation I shall, in this chapter, give a brief introduction to the density matrix formalism, and to the Hamilton and current density operators which are of central importance for a determination of the microscopic current density response. Throughout this chapter we shall make use of the Dirac notation and the state space description of quantum physics. If necessary, the reader may find an excellent introduction to the Dirac notation, the state space description, and certain aspects of the density matrix formalism in the book by Cohen-Tannoudji et al. [164].

11.1 Density Matrix Operator

11.1.1 Pure State

Let us consider a quantum physical system whose state vector at the instant t is given by

$$|\Psi(t)\rangle = \sum_n c_n(t) |u_n\rangle, \quad (11.1)$$

where the $\{|u_n\rangle\} \equiv (|u_1\rangle, |u_2\rangle, \dots |u_n\rangle, \dots)$ set forms an orthonormal basis of the state space, here, for simplicity assumed to be discrete. The $\{|u_n\rangle\}$ state vectors are associated with some physical (measurable) quantity, say $\mathcal{B}$, to which an *observable* $\hat{B}$ is associated. Hilbert space operators are in the following denoted by the same symbols as the corresponding classical quantities (if these exist), but with a caret

($\wedge$) on top. By definition, the Hermitian operator $\hat{B} = \hat{B}^\dagger$ ($\dagger$ stands for Hermitian conjugation) is an observable if its eigenvector spectrum is complete, i.e., forms a basis in the state space. For a discrete, non-degenerate spectrum, the eigenvalue problem for $\hat{B}$ is

$$\hat{B}|u_n\rangle = b_n|u_n\rangle, \quad (11.2)$$

where the b_n 's are the real eigenvalues of $\hat{B}$. Normalization of $|\Psi(t)\rangle$, i.e., the requirement $\langle\Psi(t)|\Psi(t)\rangle = 1$, implies that the coefficients $c_n(t)$ satisfy the relation

$$\sum_n |c_n(t)|^2 = 1. \quad (11.3)$$

The coefficient $c_n(t)$ is given by

$$c_n(t) = \langle u_n|\Psi(t)\rangle, \quad (11.4)$$

i.e., as the scalar product of $|u_n\rangle$ with $|\Psi(t)\rangle$ (in the shown order), as it readily follows from the orthonormality of the $|u_n\rangle$'s that is

$$\langle u_n|u_p\rangle = \delta_{np}. \quad (11.5)$$

If $\hat{A}$ is an observable, with matrix elements $\langle u_n|\hat{A}|u_p\rangle = A_{np}$ in the $\{|u_n\rangle\}$ basis, the mean value of $\hat{A}$ in the state $|\Psi(t)\rangle$ is given by

$$\langle\hat{A}\rangle(t) = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle = \sum_{n,p} c_n^*(t)c_p(t)A_{np}, \quad (11.6)$$

remembering that the scalar product between two arbitrary states $|\psi\rangle$ and $|\chi\rangle$ satisfies the relation

$$\langle\phi|\chi\rangle = \langle\chi|\phi\rangle^*. \quad (11.7)$$

Equation (11.6) shows that only quadratic expressions in the various $c_n(t)$'s enter into the mean value. Since

$$\langle u_p|\Psi(t)\rangle\langle\Psi(t)|u_n\rangle = c_p(t)c_n^*(t), \quad (11.8)$$

these quadratic expressions are the matrix elements of the operator

$$\hat{\rho}(t) \equiv |\Psi(t)\rangle\langle\Psi(t)| \quad (11.9)$$

in the $|u_n\rangle$ basis. The operator $\hat{\rho}(t)$, given by the definition in (11.9), is called the density matrix operator (or just the density operator) for the quantum state $|\Psi(t)\rangle$. If the state vector of the system is perfectly well-known at a certain initial time t_0 , i.e., $|\Psi(t_0)\rangle$ is given, the state vector of the system at an arbitrary time t in principle can be determined by solving the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle, \quad (11.10)$$

where $\hat{H}(t)$ is the Hamilton operator of the system. For a conservative system $\hat{H}$ is independent of time. A state for which the state vector $|\Psi(t)\rangle$ is known is called a *pure state*. Even if the state vector of the system is perfectly well-known *the fundamental postulate concerning the measurement process in quantum physics in general leads to probabilistic predictions*. Thus, if the physical quantity $\mathcal{B}$ is measured at time t for a system in the state $|\Psi(t)\rangle$ (11.1), the probability of $\mathcal{P}(b_n)$ of obtaining the non-degenerate eigenvalue b_n of the corresponding observable $\hat{B}$ (11.2) is given by

$$\mathcal{P}(b_n) = |\langle u_n | \Psi(t) \rangle|^2 = |c_n(t)|^2. \quad (11.11)$$

In the $\{|u_n\rangle\}$ basis, the density operator is represented by a matrix called the density matrix, whose elements are

$$\rho_{pn}(t) = \langle u_p | \hat{\rho}(t) | u_n \rangle = c_n^*(t) c_p(t). \quad (11.12)$$

By insertion of (11.12) into (11.6), the mean value of $\hat{A}$ becomes

$$\begin{aligned} \langle \hat{A} \rangle(t) &= \sum_{n,p} \langle u_p | \hat{\rho}(t) | u_n \rangle \langle u_n | \hat{A} | u_p \rangle \\ &= \sum_p \langle u_p | \hat{\rho}(t) \left[\sum_n |u_n\rangle \langle u_n| \right] \hat{A} | u_p \rangle. \end{aligned} \quad (11.13)$$

Use of the closure relation (theorem), which states that

$$\sum_n |u_n\rangle \langle u_n| = \hat{1}, \quad (11.14)$$

where $\hat{1}$ denotes the identity operator, immediately reduces (11.13) to

$$\langle \hat{A} \rangle(t) = \sum_p \langle u_p | \hat{\rho}(t) \hat{A} | u_p \rangle, \quad (11.15)$$

an equation which shows that the mean value of $\hat{A}$ can be obtained as the trace (Tr) of the operator product $\hat{\rho}\hat{A}$, i.e.,

$$\langle \hat{A} \rangle(t) = \text{Tr}\{\hat{\rho}(t)\hat{A}\}. \quad (11.16)$$

Although not stated explicitly, the operator $\hat{A}$ may of course be time dependent. If one interchanges the matrix elements of $\hat{\rho}$ and $\hat{A}$ in the first equation of (11.13) it readily appears that the mean value of $\hat{A}$ also can be written as $\langle \hat{A} \rangle(t) = \text{Tr}\{\hat{A}\hat{\rho}(t)\}$. Since $\rho_{nn}(t) = |c_n(t)|^2$, the probability conservation $d\langle \Psi(t) | \Psi(t) \rangle / dt = 0$, given

via the normalization condition in (11.3), is expressed in terms of the density operator by

$$\text{Tr}\{\hat{\rho}(t)\} = 1 \quad (11.17)$$

It follows directly from the definition in (11.9) that the density operator is Hermitian, i.e.,

$$\hat{\rho}(t) = \hat{\rho}^\dagger(t), \quad (11.18)$$

if one remembers that Hermitian conjugation of operators in the Dirac notation takes the form

$$(|\phi\rangle\langle\chi|)^\dagger = |\chi\rangle\langle\phi|. \quad (11.19)$$

For a *pure* state one also deduces from the definition of $\hat{\rho}(t)$ and the normalization of $|\Psi(t)\rangle$ that

$$\hat{\rho}^2(t) = \hat{\rho}(t), \quad (11.20)$$

and therefore

$$\text{Tr}\{\hat{\rho}^2(t)\} = 1. \quad (11.21)$$

The last two relations *only* hold for pure states. Let the (assumed) non-degenerate eigenvalue problem for the observable $\hat{A}$ be

$$\hat{A}|w_n\rangle = a_n|w_n\rangle. \quad (11.22)$$

For a system in the state $|\Psi(t)\rangle$ a measurement of $\mathcal{A}$ gives with the probability

$$\mathcal{P}(a_n) = |\langle w_n|\Psi(t)\rangle|^2 \quad (11.23)$$

the real value a_n , cf. (11.2) and (11.11). By means of the projector

$$\hat{P}_n \equiv |w_n\rangle\langle w_n| \quad (11.24)$$

one thus has $\mathcal{P}(a_n) = \langle\Psi(t)|\hat{P}_n|\Psi(t)\rangle$. A comparison of (11.6) and (11.16) in turn shows that $\mathcal{P}(a_n)$ can be calculated from the density operator as follows:

$$\mathcal{P}(a_n) = \text{Tr}\{\hat{\rho}(t)\hat{P}_n\}. \quad (11.25)$$

11.1.2 Statistical Mixture of States

In practice, the quantum state of a system is seldom perfectly determined. At a given instant the *incomplete information* we possess about the state of a system often manifests itself in the following way: The state of the system is either $|\Psi_1\rangle$ with probability p_1 , or $|\Psi_2\rangle$ with probability p_2 , etc. ... The various states $|\Psi_1\rangle$, $|\Psi_2\rangle$, ... are not necessarily orthogonal, but the associated probabilities satisfy (running index k)

$$\sum_k p_k = 1. \quad (11.26)$$

In the following it is useful to assume that the various states are normalized, i.e., $\langle \Psi_k | \Psi_k \rangle = 1$ for all k . The set $\{|\Psi_k\rangle\}$ is called a statistical mixture of states, with probabilities $\{p_k\}$. For a statistical mixture of states predictions concerning the results of measurements at a given instant hence involve two kinds of probabilities: (1) The fundamental probability associated to the uncertainty related to the quantum physical measurement process, and (2) the probability related to the incomplete information we have about the state of the system. An extension of the density matrix operator concept introduced for pure states allows one to deal with the quantum dynamics of statistical mixtures of states in an elegant fashion, as we now shall realize.

It appears from the analysis below (11.21) that *if* the state vector of the system were $|\Psi_k(t)\rangle$ at the instant t , the probability $\mathcal{P}_k(a_n)$ that a measurement of the observable $\hat{A}$ would yield the result a_n is given by

$$\mathcal{P}_k(a_n) = \text{Tr}\{\hat{\rho}_k(t) \hat{P}_n\}, \quad (11.27)$$

where

$$\hat{\rho}_k(t) = |\Psi_k(t)\rangle \langle \Psi_k(t)|. \quad (11.28)$$

To obtain for the mixture of states the probability $\mathcal{P}(a_n)$ that a measurement of $\hat{A}$ gives a_n one must weight $\mathcal{P}_k(a_n)$ by p_k and then sum over k . Thus,

$$\mathcal{P}(a_n) = \sum_k p_k \mathcal{P}_k(a_n), \quad (11.29)$$

and by insertion of (11.27)

$$\mathcal{P}(a_n) = \sum_k p_k \text{Tr}\{\hat{\rho}_k(t) \hat{P}_n\} = \text{Tr} \left\{ \left(\sum_k p_k \hat{\rho}_k(t) \right) \hat{P}_n \right\}. \quad (11.30)$$

We now define the density matrix operator $\hat{\rho}(t)$ of a statistical mixture of states by

$$\hat{\rho}(t) \equiv \sum_k p_k \hat{\rho}_k(t). \quad (11.31)$$

For a pure state, where one p_k is equal to 1, and the others 0, one regains from (11.31) the pure state density matrix operator. With the definition in (11.31) one has

$$\mathcal{P}(a_n) = \text{Tr}\{\hat{\rho}(t) \hat{P}_n\}. \quad (11.32)$$

The mean value of the observable $\hat{A}$ for a statistical mixture thus must be given by

$$\langle \hat{A} \rangle(t) = \sum_n a_n \mathcal{P}(a_n), \quad (11.33)$$

or equivalently by

$$\langle \hat{A} \rangle(t) = \text{Tr} \left\{ \hat{\rho}(t) \left(\sum_n a_n \hat{P}_n \right) \right\}. \quad (11.34)$$

Multiplication of the eigenvalue equation for $\hat{A}$ (11.22) by the bra $\langle w_n |$ from the right side gives

$$\hat{A} |w_n\rangle \langle w_n| = a_n \hat{P}_n, \quad (11.35)$$

remembering (11.24). A summation of (11.35) over all n -states, and use of the closure relation $\sum_n |w_n\rangle \langle w_n| = \hat{1}$, then lead to the following expression for $\hat{A}$:

$$\hat{A} = \sum_n a_n \hat{P}_n. \quad (11.36)$$

This relation implies that the mean value of $\hat{A}$ for a statistical mixture can be written in the form

$$\langle \hat{A} \rangle(t) = \text{Tr} \{ \hat{\rho}(t) \hat{A} \}. \quad (11.37)$$

This result represents a generalization of the formula for a pure state (11.16) to a statistical mixture of states. For the trace of $\hat{\rho}(t)$, viz.,

$$\text{Tr} \{ \hat{\rho}(t) \} = \sum_k p_k \text{Tr} \{ \hat{\rho}_k(t) \} \quad (11.38)$$

one obtains

$$\text{Tr} \{ \hat{\rho}(t) \} = 1 \quad (11.39)$$

as in the pure case, since $\text{Tr} \{ \hat{\rho}_k(t) \} = 1$ for the pure state $|\Psi_k(t)\rangle$, and $\sum_k p_k = 1$. Since $\hat{\rho}_k = \hat{\rho}_k^\dagger$ (cf. (11.19) and (11.28)) and the p_k 's are real the generalized density matrix operator in (11.31) obviously is Hermitian:

$$\hat{\rho}(t) = \hat{\rho}^\dagger(t). \quad (11.40)$$

For a pure state $|\Psi_k(t)\rangle$ with density operator $\hat{\rho}_k(t)$ we found in Sect. 11.1.1 that $\text{Tr} \{ \hat{\rho}_k^2(t) \} = 1$. In the general case of a mixture, the trace of $\hat{\rho}^2$ does not equal 1. To realize this we start from (11.37) setting $\hat{A} = \hat{\rho}$. Thus, it appears from the equation

$$\langle \hat{\rho} \rangle(t) = \text{Tr} \{ \hat{\rho}^2(t) \} \quad (11.41)$$

that the trace sought for equals the mean value of $\hat{\rho}$ for the mixture, viz.,

$$\langle \hat{\rho} \rangle = \sum_k p_k \langle \hat{\rho}_k \rangle = \sum_k p_k \sum_j p_j |\langle \Psi_j | \Psi_k \rangle|^2. \quad (11.42)$$

Since $|\langle \Psi_j | \Psi_k \rangle|^2 \leq 1$ for all pairs (j, k) of pure states in the mixture, and only equal to 1 for $j = k$, it follows that $\sum_j p_j |\langle \Psi_j | \Psi_k \rangle|^2 \leq 1$ for all k . In turn this

gives the result

$$\langle \hat{\rho} \rangle(t) \leq \sum_k p_k = 1. \quad (11.43)$$

For a statistical mixture we have thus obtained the important result

$$\text{Tr}\{\hat{\rho}^2(t)\} \leq 1. \quad (11.44)$$

Only for a pure state does the equal sign hold.

11.2 The Liouville Equation

Let us assume that a quantum system is in the pure state $|\Psi_k(t)\rangle$ at the instant t . Dynamically, the system evolves in a deterministic manner described by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi_k(t)\rangle = \hat{H}(t) |\Psi_k(t)\rangle \quad (11.45)$$

in the state vector (ket vector) space. In the dual (bra vector) space, the bra $\langle \Psi_k(t) |$ satisfies the dynamic equation

$$-i\hbar \frac{d}{dt} \langle \Psi_k(t) | = \langle \Psi_k(t) | \hat{H}(t), \quad (11.46)$$

since the Hamilton operator is an observable and therefore Hermitian, i.e.,

$$\hat{H}(t) = \hat{H}^\dagger(t). \quad (11.47)$$

The time evolution of the density matrix operator $\hat{\rho}_k(t) = |\Psi_k(t)\rangle \langle \Psi_k(t)|$ can be deduced from the Schrödinger equation. Thus, from

$$i\hbar \frac{d}{dt} \hat{\rho}_k(t) = \left(i\hbar \frac{d}{dt} |\Psi_k(t)\rangle \right) \langle \Psi_k(t) | - |\Psi_k(t)\rangle \left(-i\hbar \frac{d}{dt} \langle \Psi_k(t) | \right) \quad (11.48)$$

one obtains by insertion of (11.45) and (11.46)

$$\begin{aligned} i\hbar \frac{d}{dt} \hat{\rho}_k(t) &= \hat{H}(t) |\Psi_k(t)\rangle \langle \Psi_k(t) | - |\Psi_k(t)\rangle \langle \Psi_k(t) | \hat{H}(t) \\ &= \hat{H}(t) \hat{\rho}_k(t) - \hat{\rho}_k(t) \hat{H}(t). \end{aligned} \quad (11.49)$$

The evolution equation in (11.49) for the density matrix operator can be written in compact form with the help of the commutator concept. By definition, the commutator $[\hat{A}, \hat{B}]$ of two linear operators $\hat{A}$ and $\hat{B}$ is

$$[\hat{A}(t), \hat{B}(t)] = \hat{A}(t) \hat{B}(t) - \hat{B}(t) \hat{A}(t). \quad (11.50)$$

For a pure state $|\Psi_k(t)\rangle$, the associated density matrix operator hence satisfies the dynamical equation

$$i\hbar \frac{d}{dt} \hat{\rho}_k(t) = [\hat{H}(t), \hat{\rho}_k(t)]. \quad (11.51)$$

An equation describing the time evolution of the density matrix operator for a statistical mixture of states (11.31) now is established multiplying (11.51) by the probability p_k and carrying out thereafter a summation over k . Since the Hamilton operator is the same for all members of the statistical mixture one obtains

$$i\hbar \frac{d}{dt} \left(\sum_k p_k \hat{\rho}_k(t) \right) = [\hat{H}(t), \sum_k p_k \hat{\rho}_k(t)], \quad (11.52)$$

and, with the definition in (11.31), hence

$$i\hbar \frac{d}{dt} \hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)]. \quad (11.53)$$

Equation (11.53) often is called the Liouville equation for the density matrix operator.

In the arbitrary orthonormal basis $\{|u_n\rangle\}$, the density matrix operator is represented by numbers: Matrix elements of $\hat{\rho}$ in this basis. The numbers, which in general are time dependent, satisfy a set of coupled first-order differential equations now to be established. For the matrix elements ij we obtain from (11.53)

$$i\hbar \frac{d}{dt} \langle u_i | \hat{\rho}(t) | u_j \rangle = \langle u_i | \hat{H}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{H}(t) | u_j \rangle \quad (11.54)$$

inserting the identity operator between $\hat{H}(t)$ and $\hat{\rho}(t)$. The closure theorem (11.14) in turn gives

$$i\hbar \frac{d}{dt} \langle u_i | \hat{\rho}(t) | u_j \rangle = \sum_k \left(\langle u_i | \hat{H}(t) | u_k \rangle \langle u_k | \hat{\rho}(t) | u_j \rangle - \langle u_i | \hat{\rho}(t) | u_k \rangle \langle u_k | \hat{H}(t) | u_j \rangle \right), \quad (11.55)$$

or with the abbreviation

$$\langle u_\alpha | \hat{O}(t) | u_\beta \rangle = \mathcal{O}_{\alpha\beta}(t), \quad (11.56)$$

$$i\hbar \frac{d}{dt} \rho_{ij}(t) = \sum_k (H_{ik}(t) \rho_{kj}(t) - \rho_{ik}(t) H_{kj}(t)). \quad (11.57)$$

Equation (11.57) represents a set of coupled equations for the matrix elements of the density matrix operator. The Liouville equation for the density matrix operator is used in the calculations of various microscopic response tensors in Chap. 12.

11.3 The Configuration Space Representation

In quantum mechanics, the possibilities for measuring the position of a particle is linked to the position operator, $\hat{\mathbf{r}}$, which we assume is an observable. In the eigenvalue equation for $\hat{\mathbf{r}}$:

$$\hat{\mathbf{r}}|\mathbf{r}_0\rangle = \mathbf{r}_0|\mathbf{r}_0\rangle, \quad (11.58)$$

the state vector $|\mathbf{r}_0\rangle$ describes the quantum state of a particle definitely located at the spatial position $\mathbf{r}_0 = (x_0, y_0, z_0)$. In relativistic quantum mechanics the theory of particle position measurements is difficult and touches upon fundamental physical questions of great importance. In near-field electrodynamics, studies of the position operator problem for the photon are of central importance for the understanding of, e.g., the limitations nature sets for our ability to localize electromagnetic fields in space–time. We shall discuss the photon position operator problem briefly in Chap. 21. Below, the eigenvalue equation in (11.58) is used only for massive particles moving nonrelativistically. The state vectors $\{|\mathbf{r}_0\rangle\}$ form a continuous orthonormal basis in the extended sense. The eigenfunctions are orthonormalized in the Dirac sense, viz.,

$$\langle\mathbf{r}_0|\mathbf{r}'_0\rangle = \delta(\mathbf{r}_0 - \mathbf{r}'_0), \quad (11.59)$$

and satisfies the closure relation

$$\int |\mathbf{r}_0\rangle\langle\mathbf{r}_0|d^3r_0 = \hat{1}. \quad (11.60)$$

The representation in state space which relates to the $\{|\mathbf{r}_0\rangle\}$ basis is called the configuration space representation, or just the $\{|\mathbf{r}\rangle\}$ representation. In the $\{|\mathbf{r}_0\rangle\}$ basis the expansion of an arbitrary state vector $|\Psi(t)\rangle$ is given by

$$|\Psi(t)\rangle = \int \langle\mathbf{r}_0|\Psi(t)\rangle|\mathbf{r}_0\rangle d^3r_0, \quad (11.61)$$

as one readily realizes by means of the closure relation. The expansion coefficient

$$\langle\mathbf{r}_0|\Psi(t)\rangle \equiv \Psi(\mathbf{r}_0, t) \quad (11.62)$$

which relates to $|\mathbf{r}_0\rangle$ is just the configuration space wave function $\Psi(\mathbf{r}, t)$ at the spatial position $\mathbf{r}_0$. The set of state space kets $\{|\mathbf{r}_0\rangle\}$ is associated to the set $\{\delta(\mathbf{r}-\mathbf{r}_0)\}$ of delta functions in configuration space ($\mathbf{r}_0$ being the continuous vectorial index), i.e.,

$$\delta(\mathbf{r} - \mathbf{r}_0) \Leftrightarrow |\mathbf{r}_0\rangle. \quad (11.63)$$

The inner product

$$\langle\phi|\chi\rangle = \int_{-\infty}^{\infty} \phi^*(\mathbf{r})\chi(\mathbf{r})d^3r \quad (11.64)$$

associates state and configuration space operations, e.g.,

$$\langle \mathbf{r}_0 | \mathbf{r}'_0 \rangle = \int_{-\infty}^{\infty} \delta^*(\mathbf{r} - \mathbf{r}_0) \delta(\mathbf{r} - \mathbf{r}'_0) d^3 r = \delta(\mathbf{r}_0 - \mathbf{r}'_0), \quad (11.65)$$

and

$$\langle \mathbf{r}_0 | \Psi(t) \rangle = \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}_0) \Psi(\mathbf{r}, t) d^3 r = \Psi(\mathbf{r}_0, t). \quad (11.66)$$

The scalar product definition in (11.64) is unsatisfactory from a relativistic point of view, and the naive position operator $\hat{\mathbf{r}}$ is not Hermitian when the satisfactory Lorentz invariant scalar product is introduced. Using (11.58), (11.64), and the association in (11.63), one obtains

$$\langle \mathbf{r} | \hat{\mathbf{r}} | \mathbf{r}' \rangle = \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}'') \mathbf{r}' \delta(\mathbf{r}' - \mathbf{r}'') d^3 r'' = \mathbf{r} \delta(\mathbf{r} - \mathbf{r}'). \quad (11.67)$$

The corresponding matrix element for a function $\hat{F}(\hat{\mathbf{r}})$ of $\hat{\mathbf{r}}$ is

$$\langle \mathbf{r} | \hat{F}(\hat{\mathbf{r}}) | \mathbf{r}' \rangle = F(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'). \quad (11.68)$$

In the $\{|\mathbf{r}\rangle\}$ representation, the particle momentum operator $\hat{\mathbf{p}}$ formally acts on $|\mathbf{r}_0\rangle$ as follows:

$$\hat{\mathbf{p}} |\mathbf{r}_0\rangle = \frac{\hbar}{i} \nabla_0 |\mathbf{r}_0\rangle, \quad (11.69)$$

where ∇_0 is the gradient operator in the $\mathbf{r}_0$ -coordinates. By using (11.64), (11.69), and the prescription in (11.63), one gets

$$\langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle = \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}'') \frac{\hbar}{i} \nabla' \delta(\mathbf{r}' - \mathbf{r}'') d^3 r'' = \frac{\hbar}{i} \nabla \delta(\mathbf{r} - \mathbf{r}'), \quad (11.70)$$

and thereafter for a function $\hat{G}(\hat{\mathbf{p}})$

$$\langle \hat{\mathbf{r}} | \hat{G}(\hat{\mathbf{p}}) | \hat{\mathbf{r}}' \rangle = G\left(\frac{\hbar}{i} \nabla\right) \delta(\mathbf{r} - \mathbf{r}'). \quad (11.71)$$

How do we arrive at the Schrödinger equation in the wave function representation starting from (11.10)? First we take the inner product of (11.10) with $|\mathbf{r}\rangle$:

$$i\hbar \frac{\partial}{\partial t} \langle \mathbf{r} | \Psi(t) \rangle = \langle \mathbf{r} | \hat{H}(t) \hat{1} | \Psi(t) \rangle. \quad (11.72)$$

Then we use the closure relation (11.60) to replace the identity operator inserted above behind $\hat{H}(t)$:

$$i\hbar \frac{\partial}{\partial t} \langle \mathbf{r} | \Psi(t) \rangle = \int_{-\infty}^{\infty} \langle \mathbf{r} | \hat{H}(t) | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi(t) \rangle d^3 r'. \quad (11.73)$$

In the $\{|r\rangle\}$ representation, the Hamilton operator is a function of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, and in general t , i.e., $\hat{H} = \hat{H}(\hat{\mathbf{r}}, \hat{\mathbf{p}}, t)$, as we shall see in the next subsection. Utilizing (11.68) and (11.71) we next find (keeping for later convenience a caret on the Hamiltonian on the right side of the following equation)

$$\langle \mathbf{r} | \hat{H}(\hat{\mathbf{r}}, \hat{\mathbf{p}}, t) | \mathbf{r}' \rangle = \hat{H}(\mathbf{r}, \frac{\hbar}{i} \nabla, t) \delta(\mathbf{r} - \mathbf{r}'). \quad (11.74)$$

Since $\langle \hat{\mathbf{r}} | \Psi(t) \rangle = \Psi(\mathbf{r}, t)$, one finally obtains

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \hat{H}(\mathbf{r}, \frac{\hbar}{i} \nabla, t) \Psi(\mathbf{r}, t). \quad (11.75)$$

This is the nonrelativistic Schrödinger equation for a single particle in the configuration space representation. Since the wave function $\Psi(\mathbf{r}, t)$ is a function of the independent variables $\mathbf{r}$ and t , partial derivatives $(\partial/\partial t)$ appear in (11.72) and below. In the $\{|\hat{\mathbf{r}}\rangle\}$ representation, where $\langle \mathbf{r} | \hat{\rho}(t) | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \hat{\rho}(\mathbf{r}, -i\hbar \nabla, t)$, one has the following single-particle Liouville equation for $\hat{\rho}(\mathbf{r}, -i\hbar \nabla, t)$:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(\mathbf{r}, \frac{\hbar}{i} \nabla, t) = \left[\hat{H}(\mathbf{r}, \frac{\hbar}{i} \nabla, t), \hat{\rho}(\mathbf{r}, \frac{\hbar}{i} \nabla, t) \right], \quad (11.76)$$

as the reader herself may show.

11.4 Hamilton Operator in Minimal Coupling Form

11.4.1 The Relativistic Standard Hamiltonian

The Maxwell–Lorentz equations ((2.1)–(2.4)) and the Newton–Lorentz equation (2.30) can be derived from a general variational principle, the principle of least action. This principle expresses the stationarity of the so-called action, which is a certain time integral of the (not unique) Lagrangian of the particle–field system. The stationarity leads to establishment of the Lagrange equations, from which the fundamental equations of microscopic classical electrodynamics can be obtained. From the Lagrangian approach one may proceed to the Hamiltonian formalism by substituting for the Lagrangian another function, the Hamiltonian. From the Hamiltonian one is led to Hamilton’s equations, and from these one can also derive the Maxwell–Lorentz and Newton–Lorentz equations. The Hamiltonian approach is essential for the quantization of the classical theory, as we shall see. In relation to the later descriptions of the Hamilton–Jacobi approach to photon wave mechanics in the eikonal limit (Chap. 19) and near-field electrodynamics with quantized fields (Part III of the book), we shall briefly summarize some of the essentials of the Lagrange and Hamilton formalisms.

In the present context, it is sufficient to start from the so-called standard Lagrangian. This Lagrangian has three parts: The Lagrangian for the particles, the Lagrangian for the electromagnetic field, and the Lagrangian responsible for the field–particle interaction. To determine (1) the classical motion, and (2) the Schrödinger equation of the particles subjected to the Lorentz force, we do not need the electromagnetic field part of the Lagrangian. Leaving out this part, the relevant relativistic standard Lagrangian is for a system of spinless particles given by

$$L = \sum_{\alpha} L_{\alpha}, \quad (11.77)$$

where

$$L_{\alpha} = -\gamma_{\alpha}^{-1} m_{\alpha} c_0^2 + q_{\alpha} [\mathbf{v}_{\alpha} \cdot \mathbf{A}(\mathbf{r}_{\alpha}, t) - \phi(\mathbf{r}_{\alpha}, t)] \quad (11.78)$$

is the Lagrangian for the particle α . The notation used in (11.78) is the same as the one used in Chap. 2. The Lagrangian is a function of the sets of position coordinates $\{\mathbf{r}_{\alpha}(t)\}$ and velocities $\{\dot{\mathbf{r}}_{\alpha}(t)\} \equiv \{\mathbf{v}_{\alpha}(t)\}$, and of time t , i.e., $L = L(\{\mathbf{r}_{\alpha}\}, \{\mathbf{v}_{\alpha}\}, t)$ as one readily sees remembering that

$$\gamma_{\alpha}^{-1} = \left(1 - \frac{v_{\alpha}^2}{c_0^2}\right)^{1/2}. \quad (11.79)$$

The conjugate momentum, $\mathbf{p}_{\alpha}$, of the position $\mathbf{r}_{\alpha}$, defined by

$$\mathbf{p}_{\alpha} \equiv \nabla_{\mathbf{v}_{\alpha}} L(\{\mathbf{r}_{\alpha}\}, \{\mathbf{v}_{\alpha}\}, t), \quad (11.80)$$

is given by

$$\mathbf{p}_{\alpha} = \boldsymbol{\pi}_{\alpha} + q_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}, t), \quad (11.81)$$

as the reader may prove by an elementary calculation. The quantity $\boldsymbol{\pi}_{\alpha} = \gamma_{\alpha} m_{\alpha} \mathbf{v}_{\alpha}$ is the relativistic mechanical momentum of the particle (α) (already introduced in (9.80)), and in the *Coulomb gauge*, where $\mathbf{A} = \mathbf{A}_T$, the last term in (11.81) is the particle's electromagnetic momentum, cf. the discussion in Sect. 9.3.3. The classical Hamiltonian of the field–particle system (again with the electromagnetic field part omitted) is given by

$$H = \sum_{\alpha} H_{\alpha}, \quad (11.82)$$

where, by definition,

$$H_{\alpha} \equiv \mathbf{p}_{\alpha} \cdot \mathbf{v}_{\alpha} - L_{\alpha}(\mathbf{r}_{\alpha}, \mathbf{v}_{\alpha}, t). \quad (11.83)$$

As it stands, H_{α} is a function of both $\mathbf{v}_{\alpha}$ and $\mathbf{p}_{\alpha}$, but (11.81) allows one to eliminate $\mathbf{v}_{\alpha}$ in favor of $\mathbf{p}_{\alpha}$ so that the Hamiltonian finally appears as a function of the conjugate positions and momenta, and of time, i.e., $H = H(\{\mathbf{r}_{\alpha}\}, \{\mathbf{p}_{\alpha}\}, t)$. To determine the final form of H , we insert (11.78) into (11.83), and replace hereafter $\mathbf{v}_{\alpha}$ by $\boldsymbol{\pi}_{\alpha} \gamma_{\alpha}^{-1} m_{\alpha}^{-1}$. Thus, we obtain

$$H_\alpha = m_\alpha c_0^2 \gamma_\alpha^{-1} \left(1 + \frac{\pi_\alpha^2}{m_\alpha^2 c_0^2} \right) + q_\alpha \phi(\mathbf{r}_\alpha, t). \quad (11.84)$$

Utilizing once more the relation $\pi_\alpha = \gamma_\alpha m_\alpha \mathbf{v}_\alpha$ to express $\mathbf{v}_\alpha^2$ in terms of π_α^2 , insertion in (11.79) thereupon gives

$$\gamma_\alpha^{-1} = \left(1 + \frac{\pi_\alpha^2}{m_\alpha^2 c_0^2} \right)^{-1/2}. \quad (11.85)$$

By combining (11.84) and (11.85) we obtain the desired form

$$H_\alpha = m_\alpha c_0^2 \left[1 + m_\alpha^{-2} c_0^{-2} (\mathbf{p}_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t))^2 \right]^{1/2} + q_\alpha \phi(\mathbf{r}_\alpha, t). \quad (11.86)$$

11.4.2 Pauli and Nonrelativistic Hamiltonians

In the nonrelativistic regime, the last term under the square root sign in (11.86) is small compared to unity. Expansion to first order immediately gives, to within a constant term $\sum_\alpha m_\alpha c_0^2$, the following nonrelativistic Hamiltonian:

$$H(\{\mathbf{r}_\alpha\}, \{\mathbf{p}_\alpha\}, t) = \sum_\alpha \left[\frac{1}{2m_\alpha} (\mathbf{p}_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t))^2 + q_\alpha \phi(\mathbf{r}_\alpha, t) \right]. \quad (11.87)$$

In Chap. 20, we shall examine the electromagnetic radiation associated with a pure spin transition in order to obtain insight in certain aspects of the spatial localization problem for photons. For this purpose, we need to consider the interaction between a spin-1/2 particle and the local electromagnetic field prevailing at the particle position. Basically spin is a relativistic internal quantum property of an elementary particle, and as such it has no place in classical electrodynamics. Heuristically, one may bring the spin-field interaction on the classical scene by adding to the Hamiltonian in (11.87) terms which describe the potential energy of the various particles, each with a specific magnetic (dipole) moment, when placed in the self-consistent magnetic field prevailing in the system. To particle α we thus associate a magnetic (dipole) moment

$$\mathbf{M}_{S,\alpha} = g_\alpha \mu_{B,\alpha} \hbar^{-1} \mathbf{S}_\alpha, \quad (11.88)$$

where g_α is the so-called g -factor of the particle, and

$$\mu_{B,\alpha} = \frac{q_\alpha \hbar}{2m_\alpha} \quad (11.89)$$

is the Bohr magneton. In the present notation, the Bohr magneton can be positive or negative, depending on the electrical charge of the particle. For an electron (e),

$g_e \approx 2$. The quantity $\mathbf{S}_\alpha$ is the *spin* angular momentum of particle α . In the framework of microscopic classical electrodynamics we realized in Sect. 5.1 that the magnetic dipole moment of a particle with *orbital* angular momentum $\mathbf{L}_\alpha$ in the nonrelativistic limit was given by $\mathbf{m} = \mu_{B,\alpha} \hbar^{-1} \mathbf{L}_\alpha$ (5.27). By comparison, one thus has the transcription $\mathbf{L}_\alpha \Leftrightarrow g_\alpha \mathbf{S}_\alpha$. For an electron with $g_e \approx 2$, it thus seems impossible at first sight to classify the spin as *a kind* of orbital angular momentum. Although this is also the message in the quantum mechanical standard description, it is known [250] that the spin angular momentum *can* be interpreted as an orbital angular momentum of a particle located in a volume of linear extension comparable to the Compton wavelength, $\lambda_{C,\alpha} = h/(m_\alpha c_0)$ of the particle. By means of the dimensionless Pauli spin vector $\boldsymbol{\sigma}_\alpha$, defined via

$$\mathbf{S}_\alpha \equiv \frac{\hbar}{2} \boldsymbol{\sigma}_\alpha, \quad (11.90)$$

the magnetic spin moment is given by

$$\mathbf{M}_{S,\alpha} = \frac{g_\alpha}{2} \mu_{B,\alpha} \boldsymbol{\sigma}_\alpha. \quad (11.91)$$

The interaction of the particle spin with the selfconsistent magnetic field $\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t)$ adds a contribution

$$H^{\text{spin}} = - \sum_{\alpha} \mathbf{M}_{S,\alpha} \cdot \mathbf{B}(\mathbf{r}_\alpha(t), t) \quad (11.92)$$

to the system Hamiltonian. The sum of the contributions in (11.87) and (11.92) i.e.,

$$H = \sum_{\alpha} \left[\frac{1}{2m_\alpha} (\mathbf{p}_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t))^2 + q_\alpha \phi(\mathbf{r}_\alpha, t) - \frac{g_\alpha}{2} \mu_{B,\alpha} \boldsymbol{\sigma}_\alpha \cdot \nabla \times \mathbf{A}(\mathbf{r}_\alpha, t) \right], \quad (11.93)$$

is the so-called classical Pauli Hamiltonian for a system of spin-1/2 particles. The Hamilton operator associated to the Pauli Hamiltonian can be derived from the fully relativistic Dirac Hamiltonian operator in the limit where the relativistic effects are small.

11.4.3 Canonical Quantization

In the semiclassical (field-unquantized) quantum theory, the various conjugate position ($\mathbf{r}_\alpha$) and momentum ($\mathbf{p}_\alpha$) variables become operators, i.e.,

$$\mathbf{r}_\alpha \Rightarrow \hat{\mathbf{r}}_\alpha, \quad (11.94)$$

$$\mathbf{p}_\alpha \Rightarrow \hat{\mathbf{p}}_\alpha. \quad (11.95)$$

The Cartesian components ($i, j = x, y, z$) of these operators satisfy the fundamental commutation relations

$$[\hat{r}_{\alpha,i}, \hat{r}_{\beta,j}] = [\hat{p}_{\alpha,i}, \hat{p}_{\beta,j}] = 0, \quad (11.96)$$

$$[\hat{r}_{\alpha,i}, \hat{p}_{\beta,j}] = i\hbar\delta_{\alpha\beta}\delta_{ij}. \quad (11.97)$$

The Kronecker delta $\delta_{\alpha\beta}$ in (11.97) indicates that the conjugate variables of two different particles commute. For a given particle the components of these variables also commute unless they belong to the same Cartesian direction. In the $\{\mathbf{r}\}$ representation the eigenvalues of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are $\mathbf{r}$ and $-i\hbar\nabla$, respectively; see (11.58) and (11.69). In consequence, the matrix elements of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ are just $\mathbf{r}$ and $-i\hbar\nabla$, times a delta function, cf. (11.67) and (11.70). Since, for a single particle (index α omitted)

$$\begin{aligned} \langle \mathbf{r} | [\hat{\mathbf{r}}, \hat{\mathbf{p}}] | \Psi(t) \rangle &= \int_{-\infty}^{\infty} \langle \mathbf{r} | [\hat{\mathbf{r}}, \hat{\mathbf{p}}] | \mathbf{r}' \rangle \langle \mathbf{r}' | \Psi(t) \rangle d^3r' \\ &= \int_{-\infty}^{\infty} [\mathbf{r}, \frac{\hbar}{i}\nabla] \delta(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}', t) d^3r' = [\mathbf{r}, \frac{\hbar}{i}\nabla] \Psi(\mathbf{r}, t), \end{aligned} \quad (11.98)$$

one obtains in the configuration space representation

$$[r_i, \frac{\hbar}{i}\nabla_j] = i\hbar\delta_{ij}, \quad (11.99)$$

in agreement with (11.97). The canonical quantization procedure introduced above implies that the standard Hamilton operator for a system of relativistic spinless particles takes the following form in the $\{|\mathbf{r}\rangle\}$ representation:

$$\hat{H} = \sum_{\alpha} \left\{ m_{\alpha} c_0^2 \left[1 + m_{\alpha}^{-2} c_0^{-2} \left(\frac{\hbar}{i} \nabla_{\alpha} - q_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}, t) \right)^2 \right]^{1/2} + q_{\alpha} \phi(\mathbf{r}_{\alpha}, t) \right\}. \quad (11.100)$$

In the nonrelativistic limit, the standard Hamilton operator is given by

$$\hat{H} = \sum_{\alpha} \left[\frac{1}{2m_{\alpha}} \left(\frac{\hbar}{i} \nabla_{\alpha} - q_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}, t) \right)^2 + q_{\alpha} \phi(\mathbf{r}_{\alpha}, t) \right], \quad (11.101)$$

cf. (11.87). We say that the Hamilton operator in (11.100) is written in so-called *minimal coupling* form. By this we mean that the electrodynamic field–particle interaction is restricted to terms which (1) depend explicitly on the potentials only, and (2) do not violate gauge invariance; see Sect. 11.6.

To quantize the Pauli Hamiltonian (11.93) let us briefly consider the spin state space for a single particle (index α omitted). This space is two-dimensional for a spin-1/2 particle, and as a basis $\{|\uparrow\rangle, |\downarrow\rangle\}$, we shall take the orthonormal

eigenkets common to the square ($\hat{S}^2$) of the spin angular momentum operator ($\hat{\mathbf{S}}$), and the z -component ($\hat{S}_z$) of this operator. The spin operator $\hat{\mathbf{S}}$ is an angular momentum operator, and its three Cartesian components are observables. As an angular momentum operator the components of $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ satisfy the commutation relation

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \quad (11.102)$$

and two others which are deduced by cyclic permutation of the indices x, y and z . In compact notation, the three relations can be written in the vectorial form

$$\hat{\mathbf{S}} \times \hat{\mathbf{S}} = i\hbar\hat{\mathbf{S}}. \quad (11.103)$$

Note that the vector product $\hat{\mathbf{S}} \times \hat{\mathbf{S}}$ is not zero because the components of $\hat{\mathbf{S}}$ do not commute. The eigenvalue equations for $\hat{S}^2$ and $\hat{S}_z$ are

$$\hat{S}^2|\uparrow\rangle = \frac{3}{4}\hbar^2|\uparrow\rangle, \quad \hat{S}^2|\downarrow\rangle = \frac{3}{4}\hbar^2|\downarrow\rangle, \quad (11.104)$$

$$\hat{S}_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle, \quad \hat{S}_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle, \quad (11.105)$$

To describe the quantum state of the spin-1/2 particle completely one must combine the state space, which is isomorphic to the configuration space, and is called the orbital state space, and the spin state space. A basis in the combined state space can be obtained from the set of state vectors which is formed by all tensor products of chosen basis vectors (kets) in the orbital state space with chosen basis vectors (kets) in the spin state space. In the orbital state space we use the configuration space state vectors $\{|\mathbf{r}\rangle\}$, and in the spin state space the vectors $\{|\uparrow\rangle, |\downarrow\rangle\}$. In the combined space the basis vectors hence have the form

$$|\mathbf{r}, s\rangle \equiv |\mathbf{r}\rangle \otimes |s\rangle, \quad s = \uparrow \text{ or } \downarrow \quad (11.106)$$

The $\{|\mathbf{r}, s\rangle\}$ basis vectors are orthonormal in the extended sense

$$\langle \mathbf{r}', s' | \mathbf{r}, s \rangle = \delta_{s's} \delta(\mathbf{r}' - \mathbf{r}), \quad (11.107)$$

since the eigenfunctions $\{|\mathbf{r}\rangle\}$ are mutually orthonormalized (11.59), and the same holds for the spin-1/2 kets, i.e., $\langle s' | s \rangle = \delta_{s's}$. The $\{|\mathbf{r}, s\rangle\}$ set also satisfies a closure relation in the form

$$\int (|\mathbf{r}, \uparrow\rangle\langle \mathbf{r}, \uparrow| + |\mathbf{r}, \downarrow\rangle\langle \mathbf{r}, \downarrow|) d^3r = \hat{1}. \quad (11.108)$$

By utilizing the closure relation any state vector $|\Psi(t)\rangle = \hat{1}|\Psi(t)\rangle$ in the combined orbital-spin state space can be expanded as follows:

$$|\Psi(t)\rangle = \sum_{s=\uparrow, \downarrow} \int \langle \mathbf{r}, s | \Psi(t) \rangle |\mathbf{r}, s\rangle d^3r, \quad (11.109)$$

and $|\Psi(t)\rangle$ therefore is represented by the two spatial functions $\Psi_\uparrow(\mathbf{r}, t) \equiv \langle \mathbf{r}, \uparrow | \Psi(t) \rangle$ and $\Psi_\downarrow(\mathbf{r}, t) \equiv \langle \mathbf{r}, \downarrow | \Psi(t) \rangle$, characterizing, respectively, the spin up ($\uparrow$) and spin down ($\downarrow$) parts of the state. These two functions are usually written in the form of a *two-component spinor*:

$$\Psi(\mathbf{r}, t) = \begin{pmatrix} \langle \mathbf{r}, \uparrow | \Psi(t) \rangle \\ \langle \mathbf{r}, \downarrow | \Psi(t) \rangle \end{pmatrix} = \begin{pmatrix} \Psi_\uparrow(\mathbf{r}, t) \\ \Psi_\downarrow(\mathbf{r}, t) \end{pmatrix}. \quad (11.110)$$

In the spinor notation, the Pauli Hamiltonian (11.93) when quantized turns into a 2×2 matrix operator

$$\hat{H} = \sum_\alpha \left\{ \left[\frac{1}{2m_\alpha} \left(\frac{\hbar}{i} \nabla_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t) \right)^2 + q_\alpha \phi(\mathbf{r}_\alpha, t) \right] \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{g_\alpha}{2} \mu_{B,\alpha} \hat{\boldsymbol{\sigma}}_\alpha \cdot \nabla \times \mathbf{A}(\mathbf{r}_\alpha, t) \right\}, \quad (11.111)$$

where the Cartesian components of the Pauli spin operator for particle α , $\hat{\boldsymbol{\sigma}}_\alpha = (\hat{\sigma}_{\alpha,x}, \hat{\sigma}_{\alpha,y}, \hat{\sigma}_{\alpha,z})$, are represented by the 2×2 Pauli matrices. The operator $\hat{\boldsymbol{\sigma}}_\alpha$ *only* acts on particle α , but the Pauli matrices have the same form for every spin-1/2 particle, viz.,

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (11.112)$$

The reader may convince herself that the Pauli matrices satisfy

$$\hat{\sigma}_i \hat{\sigma}_j = i \sum_k \epsilon_{ijk} \hat{\sigma}_k + \delta_{ij} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (11.113)$$

where ϵ_{ijk} is element (ijk) of the completely antisymmetric Levi-Civita unit tensor ϵ . From (11.113) follows the vectorial commutator relation

$$\hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{\sigma}} = 2i \hat{\boldsymbol{\sigma}}, \quad (11.114)$$

which could have been deduced from (11.103) since one necessarily has $\hat{\mathbf{S}} = (\hbar/2)\hat{\boldsymbol{\sigma}}$ (cf. (11.90)). Equation (11.113) also implies that

$$\hat{\sigma}_i \hat{\sigma}_j + \hat{\sigma}_j \hat{\sigma}_i = 2\delta_{ij} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (11.115)$$

The Pauli matrices therefore anticommute with each other, i.e.,

$$\{\hat{\sigma}_i, \hat{\sigma}_j\} \equiv \hat{\sigma}_i \hat{\sigma}_j + \hat{\sigma}_j \hat{\sigma}_i = 0, \quad i \neq j. \quad (11.116)$$

When we later on, in Chap. 20, discuss the photon emission and localization associated with a pure spin transition the Pauli theory will be used.

11.5 Orbital Probability Current Density

In the present section, the probability current density of a nonrelativistic spinless particle interacting with an electromagnetic field is studied, and an expression for the associated Hermitian current density operator is derived. The current density which is related to the spin dynamics in the Pauli theory is discussed in Chap. 20. Once the probability current density of a single particle has been obtained, the total current density of a system of particles is easily determined (as the sum of the individual particle current densities).

11.5.1 Probability Current Density in Wave Function Space

To find an expression for the quantum mechanical current density one seeks to establish a local conservation law for the probability. We know that the probability density is given by $|\Psi(\mathbf{r}, t)|^2$, where $\Psi(\mathbf{r}, t)$ satisfies the nonrelativistic Schrödinger equation in (11.75). For a particle with charge q , the related electric (electromagnetic) probability density therefore is

$$\rho(\mathbf{r}, t) = q|\Psi(\mathbf{r}, t)|^2 \quad (11.117)$$

Let us multiply (11.75) by $\Psi^*(\mathbf{r}, t)$, and then subtract from the resulting equation its complex conjugate. This gives

$$i\hbar \frac{\partial}{\partial t} |\Psi|^2 = \Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^*, \quad (11.118)$$

where

$$\hat{H} = \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 + q\phi. \quad (11.119)$$

If one writes the Hamilton operator and its complex conjugate in the forms

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{q^2}{2m} \mathbf{A}^2 + q\phi + \frac{i\hbar q}{2m} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla), \quad (11.120)$$

$$\hat{H}^* = -\frac{\hbar^2}{2m} \nabla^2 + \frac{q^2}{2m} \mathbf{A}^2 + q\phi - \frac{i\hbar q}{2m} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla), \quad (11.121)$$

and remembers that the operator $\nabla \cdot \mathbf{A}$ when operating on Ψ gives $\nabla \cdot (\mathbf{A}\Psi)$, the right side of (11.118) can be written as follows:

$$\begin{aligned} \Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^* &= -\frac{\hbar^2}{2m} (\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*) \\ &+ \frac{i\hbar q}{2m} [\Psi^* \nabla \cdot (\mathbf{A} \Psi) + \Psi \mathbf{A} \cdot \nabla \Psi^* + \Psi \nabla \cdot (\mathbf{A} \Psi^*) + \Psi^* \mathbf{A} \cdot \nabla \Psi]. \end{aligned} \quad (11.122)$$

By means of the vector identity $\nabla \cdot (\nu \nabla V) = (\nabla \nu) \cdot (\nabla V) + \nu \nabla^2 V$, (11.122) is transformed to

$$\Psi^* \hat{H} \Psi - \Psi \hat{H}^* \Psi^* = -\frac{\hbar^2}{2m} \nabla \cdot (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) + \frac{i\hbar q}{2m} \nabla \cdot (\Psi^* \mathbf{A} \Psi + \Psi \mathbf{A} \Psi^*). \quad (11.123)$$

By combination of (11.118) and (11.123) one obtains after a few rearrangements

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \frac{\partial}{\partial t} \rho(\mathbf{r}, t) = 0, \quad (11.124)$$

where

$$\begin{aligned} \mathbf{J}(\mathbf{r}, t) &= \frac{q}{2m} \left[\Psi^*(\mathbf{r}, t) \left(\frac{\hbar}{i} \nabla - q \mathbf{A}(\mathbf{r}, t) \right) \Psi(\mathbf{r}, t) \right. \\ &\quad \left. + \Psi(\mathbf{r}, t) \left(-\frac{\hbar}{i} \nabla - q \mathbf{A}(\mathbf{r}, t) \right) \Psi^*(\mathbf{r}, t) \right] \\ &= \frac{q}{m} \Re \left\{ \Psi^*(\mathbf{r}, t) \left(\frac{\hbar}{i} \nabla - q \mathbf{A}(\mathbf{r}, t) \right) \Psi(\mathbf{r}, t) \right\}. \end{aligned} \quad (11.125)$$

The relation in (11.124) expresses the local conservation of charge in the probabilistic sense, and $\mathbf{J}(\mathbf{r}, t)$ in (11.125) can be interpreted as the electric (electromagnetic) probability current density of a particle placed in an electromagnetic field.

11.5.2 Para- and Diamagnetic Current Densities

It is often convenient to divide the probability current density into two parts, viz.,

$$\mathbf{J}(\mathbf{r}, t) = \mathbf{J}_0(\mathbf{r}, t) + \mathbf{J}_A(\mathbf{r}, t), \quad (11.126)$$

where

$$\mathbf{J}_0(\mathbf{r}, t) = \frac{q\hbar}{2mi} (\Psi^*(\mathbf{r}, t) \nabla \Psi(\mathbf{r}, t) - \Psi(\mathbf{r}, t) \nabla \Psi^*(\mathbf{r}, t)), \quad (11.127)$$

and

$$\mathbf{J}_A(\mathbf{r}, t) = -\frac{q^2}{m} \mathbf{A}(\mathbf{r}, t) |\Psi(\mathbf{r}, t)|^2. \quad (11.128)$$

The $\mathbf{J}_0$ -term, which does not depend explicitly on the vector potential, is sometimes called the paramagnetic probability current density. The $\mathbf{J}_A$ -term, which explicit dependence on $\mathbf{A}$ is linear, is often called the diamagnetic probability current density. The division in (11.126) contains a certain arbitrariness since the two terms are not gauge invariant; see Sect. 11.6. The sum of the terms is gauge invariant, however, and only the total current density relates to physically observable quantities. In this book, we usually shall reserve the names paramagnetic and diamagnetic for a slightly different division of the probability current density. The diamagnetic (dia) current density defined by

$$\mathbf{J}^{\text{dia}}(\mathbf{r}, t) = -\frac{q^2}{m} \mathbf{A}_T(\mathbf{r}, t) |\Psi(\mathbf{r}, t)|^2 \quad (11.129)$$

thus contains only the transverse part of the vector potential. The remaining part of the total probability current density is called the paramagnetic (par) part. This part is given by

$$\mathbf{J}^{\text{par}}(\mathbf{r}, t) = \frac{q\hbar}{2mi} (\Psi^*(\mathbf{r}, t) \nabla \Psi(\mathbf{r}, t) - \Psi(\mathbf{r}, t) \nabla \Psi^*(\mathbf{r}, t)) - \frac{q^2}{m} \mathbf{A}_L(\mathbf{r}, t) |\Psi(\mathbf{r}, t)|^2, \quad (11.130)$$

and deviates from $\mathbf{J}_0(\mathbf{r}, t)$ by a term which depends explicitly on the longitudinal part of the vector potential. The current densities $\mathbf{J}^{\text{dia}}(\mathbf{r}, t)$ and $\mathbf{J}^{\text{par}}(\mathbf{r}, t)$ are both gauge invariant quantities as we shall realize later on, and observable phenomena are attached to each of the two terms. The Meissner effect in BCS superconductivity thus is connected to $\mathbf{J}^{\text{dia}}(\mathbf{r}, t)$ [98, 280, 281], and in photon wave mechanics transverse photons become massive in their high-frequency interaction with matter because of $\mathbf{J}^{\text{dia}}(\mathbf{r}, t)$ cf. the discussion in Sect. 19.2. From a physical point of view the division $\mathbf{J} = \mathbf{J}^{\text{dia}} + \mathbf{J}^{\text{par}}$ therefore plays an important role. In the Coulomb gauge, $\mathbf{J}_0 = \mathbf{J}^{\text{par}}$ and $\mathbf{J}_A = \mathbf{J}^{\text{dia}}$.

11.5.3 Transition Current Density

Let us assume that the instantaneous quantum state of a nonrelativistic charged particle is given by the state vector $|\Psi(t)\rangle$ in (11.1). In the configuration space description the wave function of the particle hence is

$$\langle \mathbf{r} | \Psi(t) \rangle = \sum_i c_i(t) \langle \mathbf{r} | u_i \rangle, \quad (11.131)$$

or equivalently

$$\Psi(\mathbf{r}, t) = \sum_i c_i(t) u_i(\mathbf{r}), \quad (11.132)$$

where the orthonormal and discrete set $\{u_i(\mathbf{r})\} = \{\langle \mathbf{r} | u_i \rangle\}$ of time independent functions constitutes a basis. By insertion of (11.132) into (11.125) it readily appears that the probability current density can be written in the form

$$\mathbf{J}(\mathbf{r}, t) = \sum_{i,j} c_i(t) c_j^*(t) \mathbf{j}_{i \rightarrow j}(\mathbf{r}, t), \quad (11.133)$$

where

$$\mathbf{j}_{i \rightarrow j}(\mathbf{r}, t) = \frac{q\hbar}{2mi} (u_j^*(\mathbf{r}) \nabla u_i(\mathbf{r}) - u_i(\mathbf{r}) \nabla u_j^*(\mathbf{r})) - \frac{q^2}{m} \mathbf{A}(\mathbf{r}, t) u_i(\mathbf{r}) u_j^*(\mathbf{r}) \quad (11.134)$$

is the so-called transition current density *from* quantum state i *to* state j . When a particle makes a quantum transition from a state i to a state j , an associated probability current density distribution $c_i(t) c_j^*(t) \mathbf{j}_{i \rightarrow j}(\mathbf{r}, t)$ is generated in order to change the probability distribution from $|u_i(\mathbf{r})|^2$ to $|u_j(\mathbf{r})|^2$ (Fig. 11.1). The current density is present until the quantum transition $i \rightarrow j$ with certainty has taken place. Roughly speaking, the current density $c_i c_j^* \mathbf{j}_{i \rightarrow j}$ is located in the region of space where the orbital product $u_i u_j$ is nonvanishing. In near-field electrodynamics, the transverse part of the transition current density plays an important role for our understanding of the spatial localization of photons emitted from a given transition. Although the transition current density $\mathbf{j}_{i \rightarrow j}$, in general, is time dependent, the term proportional to the local vector potential often is negligible. In such cases $\mathbf{j}_{i \rightarrow j}$ is independent of time.

11.5.4 Orbital Current Density Operator

The canonical quantization procedure implies that the classical relation between the mechanical and canonical momenta translates into an operator equation

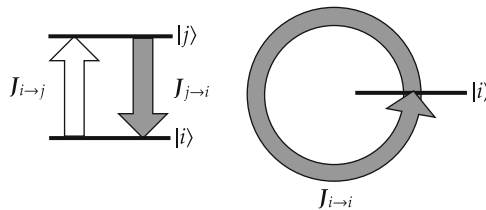


Fig. 11.1 When a particle is excited from a stationary quantum state $|i\rangle$ to a state $|j\rangle$, a transition current density distribution $\mathbf{j}_{i \rightarrow j}$ is generated in the particle domain. In the opposite ($j \rightarrow i$) transition a current density $\mathbf{j}_{j \rightarrow i} (= \mathbf{j}_{i \rightarrow j}^*)$ arises. The diamagnetic field–matter interaction always gives rise to an “internal” current density $\mathbf{j}_{i \rightarrow i}$ in the individual $|i\rangle$ -levels. If the wave function of the state $|i\rangle$ is (chosen as) real the paramagnetic interaction does not contribute to $\mathbf{j}_{i \rightarrow i}$

$$\hat{\pi} = \frac{\hbar}{i} \nabla - q \mathbf{A}(\mathbf{r}, t) \quad (11.135)$$

in the $|\mathbf{r}\rangle$ representation. In terms of the mechanical (kinematical) momentum operator $\hat{\pi}$, the probability current density takes the form

$$\mathbf{J}(\mathbf{r}, t) = \frac{q}{2m} (\Psi^*(\mathbf{r}, t) \hat{\pi} \Psi(\mathbf{r}, t) + \Psi(\mathbf{r}, t) \hat{\pi}^* \Psi^*(\mathbf{r}, t)). \quad (11.136)$$

The mechanical momentum operator is Hermitian, i.e.,

$$\hat{\pi} = \hat{\pi}^\dagger, \quad (11.137)$$

since $\hat{p} = \hat{p}^\dagger$, and $\mathbf{A}$ necessarily is real. The form of the probability current density in (11.136) indicates that the orbital probability current density is linked to a state space operator

$$\hat{j}(t) = \frac{q}{2m} [|\mathbf{r}\rangle \langle \mathbf{r}| \hat{\pi} + \hat{\pi} |\mathbf{r}\rangle \langle \mathbf{r}|]. \quad (11.138)$$

The operator $\hat{j}(t)$ is a suitably symmetrized [164] Hermitian operator formed by the charge projection operator $q|\mathbf{r}\rangle \langle \mathbf{r}|$ and the velocity operator $\hat{\pi}/m = (\hat{p} - q\mathbf{A})/m$. The mean value of $\hat{j}(t)$ in the state $|\Psi(t)\rangle$, namely,

$$\mathbf{J}(\mathbf{r}, t) = \langle \Psi(t) | \hat{j}(t) | \Psi(t) \rangle \quad (11.139)$$

is precisely equal to the probability current density in (11.136), as the reader may convince herself of using the relations $\langle \mathbf{r} | \Psi(t) \rangle = \Psi(\mathbf{r}, t)$ and $\langle \mathbf{r} | \hat{\pi} | \Psi(t) \rangle = (\frac{\hbar}{i} \nabla - q\mathbf{A})\Psi(\mathbf{r}, t)$. In wave function space the mean value of the symmetrized current density operator

$$\hat{j}(\mathbf{r}, t) = \frac{q}{2m} [\delta(\mathbf{r} - \mathbf{r}_q) \hat{\pi}(\mathbf{r}_q) + \hat{\pi}(\mathbf{r}_q) \delta(\mathbf{r} - \mathbf{r}_q)], \quad (11.140)$$

also gives the probability current density in (11.136), i.e.,

$$\mathbf{J}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \Psi^*(\mathbf{r}_q, t) \hat{j}(\mathbf{r}, t) \Psi(\mathbf{r}_q, t) d^3 r_q. \quad (11.141)$$

In (11.140) and (11.141), the vectorial particle integration variable is named $\mathbf{r}_q$. The result in (11.141) can be proved easily using the fact that the kinematic momentum operator is Hermitian. Thus,

$$\begin{aligned} \frac{q}{2m} \int_{-\infty}^{\infty} \Psi^* (\delta \hat{\pi} + \hat{\pi} \delta) \Psi d^3 r_q &= \frac{q}{2m} \int_{-\infty}^{\infty} [\Psi^* \hat{\pi} \Psi + (\hat{\pi} \Psi)^* \Psi] \delta(\mathbf{r} - \mathbf{r}_q) d^3 r_q \\ &= \mathbf{J}(\mathbf{r}, t), \end{aligned} \quad (11.142)$$

q.e.d.

11.6 Gauge Invariance in Quantum Mechanics

11.6.1 Transformation of the Mechanical Momentum Operator

As mentioned in Sect. 11.4.1, it is known that the Maxwell–Lorentz equations can be derived from Hamilton’s equations. In classical electrodynamics, the position $\mathbf{r}$ and the mechanical momentum $\boldsymbol{\pi}$ are, at every instant, gauge independent quantities that is in the notation of (2.11) and (2.12)

$$\mathbf{r}(t) \Rightarrow \mathbf{r}'(t) = \mathbf{r}(t), \quad (11.143)$$

$$\boldsymbol{\pi}(t) \Rightarrow \boldsymbol{\pi}'(t) = \boldsymbol{\pi}(t). \quad (11.144)$$

From (11.81) (index α omitted) it now follows that the canonical momenta in the two gauges are related via

$$\mathbf{p}'(t) - q\mathbf{A}'(\mathbf{r}'(t), t) = \mathbf{p}(t) - q\mathbf{A}(\mathbf{r}(t), t). \quad (11.145)$$

With the gauge transformation formula for the vector potential (2.11) inserted, and in the view of (11.143), it appears that the canonical momentum transforms according to

$$\mathbf{p}(t) \Rightarrow \mathbf{p}'(t) = \mathbf{p}(t) + q\nabla\chi(\mathbf{r}(t), t). \quad (11.146)$$

The canonical quantization principle states that the quantization rules ((11.94)–(11.97)) are the same in all gauges. In the $\{|\mathbf{r}\rangle\}$ representation we therefore have

$$\hat{\mathbf{r}}' = \hat{\mathbf{r}} = \mathbf{r}, \quad (11.147)$$

$$\hat{\mathbf{p}}' = \hat{\mathbf{p}} = \frac{\hbar}{i}\nabla, \quad (11.148)$$

The operator associated with the mechanical momentum in consequence depends on the gauge chosen. Thus,

$$\hat{\boldsymbol{\pi}}' = \hat{\boldsymbol{\pi}} - q\nabla\chi(\mathbf{r}, t), \quad (11.149)$$

and

$$\hat{\boldsymbol{\pi}} = \frac{\hbar}{i}\nabla - q\mathbf{A}(\mathbf{r}, t). \quad (11.150)$$

Similarly, the mechanical orbital angular momentum operator $\hat{\mathbf{A}}$ and the Hamilton operator are gauge dependent, i.e.,

$$\hat{\mathbf{A}} \equiv \hat{\mathbf{r}} \times \hat{\boldsymbol{\pi}} \neq \hat{\mathbf{A}}', \quad (11.151)$$

$$\hat{H} = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}}, t))^2 + q\phi(\hat{\mathbf{r}}, t) \neq \hat{H}'. \quad (11.152)$$

The usual orbital angular momentum operator

$$\hat{\mathbf{L}} \equiv \hat{\mathbf{r}} \times \hat{\mathbf{p}} \quad (11.153)$$

is the same in all gauges but it is not an observable in general. The mechanical orbital momentum operator

$$\hat{\mathbf{A}} \equiv \hat{\mathbf{L}} - q\hat{\mathbf{r}} \times \mathbf{A}(\hat{\mathbf{r}}, t) \quad (11.154)$$

is always an observable.

11.6.2 Unitary Transformation of the State Vector

In the framework of classical electrodynamics, it was realized that the canonical momentum transforms according to (11.146) under a gauge transformation given by a gauge function $\chi(\mathbf{r}, t)$. Brute force transformation of (11.146) to the quantum domain would give

$$\hat{\mathbf{p}} \Rightarrow \hat{\mathbf{p}}' \stackrel{?}{=} \hat{\mathbf{p}} + q\nabla\chi(\hat{\mathbf{r}}, t). \quad (11.155)$$

How can such a relation be in agreement with the canonical quantization principle $\hat{\mathbf{p}}' = \hat{\mathbf{p}}$ (11.148) for $\chi \neq 0$? The answer to this question lies in the fact that the analogue of the classical relation in (11.146) is *not* such a strong requirement as the one given in (11.155) between the operators. What must be fulfilled, however, is the equality of the quantum mechanical mean values in the two gauges, i.e.,

$$\langle \Psi'(t) | \hat{\mathbf{p}}' | \Psi'(t) \rangle = \langle \Psi(t) | \hat{\mathbf{p}} + q\nabla\chi(\hat{\mathbf{r}}, t) | \Psi(t) \rangle. \quad (11.156)$$

Since $\hat{\mathbf{p}}' = \hat{\mathbf{p}}$, this requirement can also be written in the form

$$\langle \Psi'(t) | \hat{\mathbf{p}} | \Psi'(t) \rangle = \langle \Psi(t) | \hat{\mathbf{p}} + q\nabla\chi(\hat{\mathbf{r}}, t) | \Psi(t) \rangle. \quad (11.157)$$

To satisfy (11.157) it is necessary that the state vectors $|\Psi(t)\rangle$ and $|\Psi'(t)\rangle$ in the two gauges are different.

We expect that the relation between the two kets depends on the gauge function operator $\chi(\hat{\mathbf{r}}, t)$. To determine this connection one seeks an operator $\hat{T}_\chi(t)$ which enables us to transform to $|\Psi(t)\rangle$ into $|\Psi'(t)\rangle$:

$$|\Psi'(t)\rangle = \hat{T}_\chi(t) |\Psi(t)\rangle. \quad (11.158)$$

Conservation of the norms of $|\Psi(t)\rangle$ and $|\Psi'(t)\rangle$, i.e.,

$$\langle \Psi'(t) | \Psi'(t) \rangle = \langle \Psi(t) | \hat{T}_\chi^\dagger(t) \hat{T}_\chi(t) | \Psi(t) \rangle = \langle \Psi(t) | \Psi(t) \rangle, \quad (11.159)$$

implies that the transformation $\hat{T}_\chi(t)$ must satisfy the operator equation

$$\hat{T}_\chi^\dagger(t)\hat{T}_\chi(t) = \hat{1}. \quad (11.160)$$

By definition, an operator $\mathcal{O}$ is unitary if its inverse $\mathcal{O}^{-1}$ is equal to its adjoint (Hermitian conjugate) $\mathcal{O}^\dagger$:

$$\hat{\mathcal{O}}^{-1} = \hat{\mathcal{O}}^\dagger. \quad (11.161)$$

From (11.161) one obtains

$$\hat{\mathcal{O}}^\dagger \hat{\mathcal{O}} = \hat{\mathcal{O}} \hat{\mathcal{O}}^\dagger = \hat{1}. \quad (11.162)$$

A comparison of (11.160) and (11.162) shows that the transformation operator $\hat{T}_\chi(t)$ must be unitary that is

$$\hat{T}_\chi^{-1}(t) = \hat{T}_\chi^\dagger(t). \quad (11.163)$$

It is useful now to write $\hat{T}_\chi(t)$ in the form

$$\hat{T}_\chi(t) = \exp\left(i\hat{F}_\chi(t)\right), \quad (11.164)$$

where $\hat{F}_\chi(t) = \hat{F}_\chi^\dagger(t)$ is an Hermitian operator. The Hermiticity of $\hat{F}_\chi(t)$ ensures that $\hat{T}_\chi(t)$ is unitary, since $\hat{T}_\chi^\dagger(t)\hat{T}_\chi(t) = \exp\left(-i\hat{F}_\chi(t)\right)\exp\left(i\hat{F}_\chi(t)\right) = \hat{1}$. Additional information on $\hat{F}_\chi(t)$ can be obtained noting that the classical requirement in (11.143) gives the following relation between the quantum mechanical mean values of the position operators (11.147) in the two gauges:

$$\langle\Psi'(t)|\hat{\mathbf{r}}|\Psi'(t)\rangle = \langle\Psi(t)|\hat{\mathbf{r}}|\Psi(t)\rangle. \quad (11.165)$$

By insertion of (11.158), and its corresponding bra ket relation into (11.165) one obtains the operator identity

$$\hat{T}_\chi^\dagger(t)\hat{\mathbf{r}}\hat{T}_\chi(t) = \hat{\mathbf{r}} \quad (11.166)$$

since the mean value relation in (11.165) must hold for any $|\Psi(t)\rangle$. Multiplying (11.166) from the left with $\hat{T}_\chi(t)$ gives the commutator relation

$$\left[\hat{\mathbf{r}}, \hat{T}_\chi(t)\right] = 0. \quad (11.167)$$

The relation in (11.167) can be satisfied if $\hat{T}_\chi(t)$ is independent of $\hat{\mathbf{p}}$. We do however expect that $\hat{T}_\chi(t)$ depends on $\hat{\mathbf{r}}$. In view of (11.164) we hence write $\hat{T}_\chi(t)$ in the form

$$\hat{T}_\chi(t) = \exp(iF_\chi(\hat{\mathbf{r}}, t)). \quad (11.168)$$

A combination of (11.157) and (11.158) leads readily to the operator relation

$$\hat{T}_\chi^\dagger(t) \hat{\mathbf{p}} \hat{T}_\chi(t) = \hat{\mathbf{p}} + q \nabla \chi(\hat{\mathbf{r}}, t), \quad (11.169)$$

or equivalently

$$\left[\hat{\mathbf{p}}, \hat{T}_\chi(t) \right] = q \hat{T}_\chi(t) \nabla \chi(\hat{\mathbf{r}}, t). \quad (11.170)$$

The commutator in (11.170) may be obtained using the fact that

$$\left[\frac{\hbar}{i} \nabla, e^{iF(\mathbf{r}, t)} \right] = \hbar e^{iF(\mathbf{r}, t)} \nabla F(\mathbf{r}, t) \quad (11.171)$$

in the $\{|\mathbf{r}\rangle\}$ representation. We are therefore necessarily led to the result

$$\hbar \nabla F(\hat{\mathbf{r}}, t) = q \nabla \chi(\hat{\mathbf{r}}, t), \quad (11.172)$$

and hence

$$F(\hat{\mathbf{r}}, t) = F_0(t) + \frac{q}{\hbar} \chi(\hat{\mathbf{r}}, t). \quad (11.173)$$

Since the multiplication of a ket by a global phase factor $\exp(iF_0(t))$ is of no physical importance the transformation operator $\hat{T}_\chi(t)$ connecting the state vectors in two gauges related by the gauge function χ hence becomes

$$\hat{T}_\chi(t) = \exp\left(i \frac{q}{\hbar} \chi(\hat{\mathbf{r}}, t)\right). \quad (11.174)$$

In the $\{|\hat{\mathbf{r}}\rangle\}$ representation, the wave function in the two gauges, namely, $\Psi(\mathbf{r}, t) = \langle \mathbf{r} | \Psi(t) \rangle$ and $\Psi'(\mathbf{r}, t) = \langle \mathbf{r} | \Psi'(t) \rangle$, are related by

$$\Psi'(\mathbf{r}, t) = \exp\left(i \frac{q}{\hbar} \chi(\mathbf{r}, t)\right) \Psi(\mathbf{r}, t). \quad (11.175)$$

For the wavefunction a gauge transformation given by $\chi(\mathbf{r}, t)$ thus corresponds to a local phase change $q\chi(\mathbf{r}, t)/\hbar$, i.e., a phase change which varies from one point to another. If one has a system containing several particles, the transformation operator is a product of the individual particle transformation operators:

$$\hat{T}_\chi(t) = \prod_\alpha \hat{T}_{\chi, \alpha}(t) = \exp \left[\frac{i}{\hbar} \sum_\alpha q_\alpha \chi(\hat{\mathbf{r}}_\alpha, t) \right]. \quad (11.176)$$

11.6.3 Form Invariance of the Schrödinger Equation

In quantum mechanics, a gauge transformation of the electromagnetic potentials ((2.11) and (2.12)) must be accompanied by a unitary transformation of the state vector ((11.158) and (11.174)). Together, these two transformations result in a form

invariance of the Schrödinger equation, as we shall prove now. Let us, thus, assume that the state vector in a gauge indicated by apostrophes satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi'(t)\rangle = \hat{H}'(t) |\Psi'(t)\rangle \quad (11.177)$$

with a Hamilton operator given by

$$\hat{H}'(t) = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}'(\hat{\mathbf{r}}, t))^2 + q\phi'(\hat{\mathbf{r}}, t), \quad (11.178)$$

cf. (11.147) and (11.148). By means of (11.158) the Schrödinger equation in (11.177) can be written

$$i\hbar \frac{d}{dt} (\hat{T}_\chi(t) |\Psi(t)\rangle) = \hat{H}'(t) \hat{T}_\chi(t) |\Psi(t)\rangle. \quad (11.179)$$

Since the gauge function $\chi(\hat{\mathbf{r}}, t)$ and the unitary operator $\hat{T}_\chi(t)$ both depend on $\hat{\mathbf{r}}$ (and not on $\hat{\mathbf{p}}$), $\partial\chi(\hat{\mathbf{r}}, t)/\partial t$ and $\hat{T}_\chi(t)$ commute. Upon differentiation, the left-hand side of (11.179) therefore becomes

$$i\hbar \frac{d}{dt} (\hat{T}_\chi(t) |\Psi(t)\rangle) = \hat{T}_\chi(t) \left(i\hbar \frac{d}{dt} |\Psi(t)\rangle \right) - q \frac{\partial\chi(\hat{\mathbf{r}}, t)}{\partial t} \hat{T}_\chi(t) |\Psi(t)\rangle. \quad (11.180)$$

By inserting (11.180) into (11.179), one obtains

$$\hat{T}_\chi(t) \left(i\hbar \frac{d}{dt} |\Psi(t)\rangle \right) = \left(\hat{H}'(t) + q \frac{\partial}{\partial t} \chi(\hat{\mathbf{r}}, t) \right) \hat{T}_\chi(t) |\Psi(t)\rangle, \quad (11.181)$$

and then after a multiplication from the left by $\hat{T}_\chi^\dagger(t)$

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \left(\hat{T}_\chi^\dagger(t) \hat{H}'(t) \hat{T}_\chi(t) + q \frac{\partial}{\partial t} \chi(\hat{\mathbf{r}}, t) \right) |\Psi(t)\rangle, \quad (11.182)$$

since $\hat{T}_\chi^\dagger \hat{T}_\chi = \hat{1}$ and $\hat{T}_\chi^\dagger (\partial\chi/\partial t) \hat{T}_\chi = \partial\chi/\partial t$. Equation (11.182) is the Schrödinger equation in the unprimed gauge provided we can prove that

$$\hat{H}(t) = \hat{T}_\chi^\dagger(t) \hat{H}'(t) \hat{T}_\chi(t) + q \frac{\partial}{\partial t} \chi(\hat{\mathbf{r}}, t). \quad (11.183)$$

To this end, we start from the relation

$$\hat{T}_\chi^\dagger (\hat{\mathbf{p}} - q\mathbf{A}')^2 \hat{T}_\chi = \hat{T}_\chi^\dagger (\hat{\mathbf{p}} - q\mathbf{A}') \hat{T}_\chi \hat{T}_\chi^\dagger (\hat{\mathbf{p}} - q\mathbf{A}') \hat{T}_\chi. \quad (11.184)$$

Utilizing first (11.169), and then the gauge transformation of the vector potential (2.11), we obtain

$$\hat{T}_\chi^\dagger (\hat{\mathbf{p}} - q\mathbf{A}')^2 \hat{T}_\chi = (\hat{\mathbf{p}} + q\nabla\chi - q\mathbf{A}')^2 = (\hat{\mathbf{p}} - q\mathbf{A})^2. \quad (11.185)$$

It follows from (11.185) that the transformation of the kinetic energy operator by the unitary transformation i.e.,

$$\hat{T}_\chi^\dagger(t) \frac{(\hat{\mathbf{p}} - q\mathbf{A}'(\hat{\mathbf{r}}, t))^2}{2m} \hat{T}_\chi(t) = \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}}, t))^2, \quad (11.186)$$

corresponds to a change from the primed to the unprimed gauge. Since the scalar potential does not depend on $\hat{\mathbf{p}}$ one has

$$\hat{T}_\chi^\dagger(t) \phi'(\hat{\mathbf{r}}, t) \hat{T}_\chi(t) = \phi'(\hat{\mathbf{r}}, t), \quad (11.187)$$

and $\phi'(\hat{\mathbf{r}}, t)$ therefore is unaffected by the unitary transformation. By adding the term $\partial\chi/\partial t$ to the two sides of (11.187) one gets in view of (2.12)

$$q \left(\hat{T}_\chi^\dagger(t) \phi'(\hat{\mathbf{r}}, t) \hat{T}_\chi(t) + \frac{\partial}{\partial t} \chi(\hat{\mathbf{r}}, t) \right) = q \phi(\hat{\mathbf{r}}, t). \quad (11.188)$$

When the results in (11.186) and (11.188) are inserted on the right-hand side of (11.183) one obtains precisely $\hat{H}(t)$. In the special case where the electromagnetic field is time independent the total energy of the particle is a constant of the motion. Since the scalar and vector potentials are also time independent in this particular case it follows that $\partial\chi/\partial t = 0$. A time independent unitary transformation $\hat{T}_\chi$ then relates the Hamilton operator in the two gauges, i.e.,

$$\hat{H} = \exp\left(-i\frac{q}{\hbar}\chi(\hat{\mathbf{r}})\right) \hat{H}' \exp\left(i\frac{q}{\hbar}\chi(\hat{\mathbf{r}})\right). \quad (11.189)$$

In a time independent electromagnetic field the Hamilton operator is a true physical observable, related to the total energy of the particle.

11.6.4 Electromagnetic Forces and Local Phase Invariance

The findings of the previous subsection can be summarized in the statement that the gauge invariance of the Maxwell–Lorentz equations remains an invariance in quantum mechanics provided a certain unitary transformation is made on the state vector. Using four-vector notation $\{A^\mu\} = (\phi/c_0, \mathbf{A})$, $\{\partial^\mu\} = (-c_0^{-1}\partial/\partial t, \nabla)$, $\mu = 0, 1, 2, 3$ the combined transformation with gauge function χ is as follows:

$$\{A^\mu\} \Rightarrow \{(A^\mu)'\} = \{A^\mu\} + \{\partial^\mu\chi\}, \quad (11.190)$$

$$|\Psi\rangle \Rightarrow |\Psi'\rangle = \exp\left(i\frac{q}{\hbar}\chi\right)|\Psi\rangle. \quad (11.191)$$

Elementary quantum mechanics has told us that a *global* phase factor does not affect any physical predictions in quantum mechanics; only relative phases of the expansion coefficients of a general state vector (11.1) play a role. Let us now be more restrictive in our demands and require that our quantum theory with classical fields be invariant under *local* phase transformations, i.e., transformations of the type in (11.191), where $\chi(\hat{\mathbf{r}}, t)$ is an arbitrary operator (function) of $\hat{\mathbf{r}}$ and t . Starting from the *free particle* Schrödinger equation

$$\frac{\hat{\mathbf{p}}^2}{2m}|\Psi(t)\rangle = i\hbar \frac{d}{dt}|\Psi(t)\rangle, \quad (11.192)$$

the transformation in (11.191) of course results in a new equation for $|\Psi'(t)\rangle$:

$$\left[\frac{1}{2m} (\hat{\mathbf{p}} - q\nabla\chi)^2 - q\frac{\partial\chi}{\partial t} \right] |\Psi'(t)\rangle = i\hbar \frac{d}{dt} |\Psi'(t)\rangle. \quad (11.193)$$

The free particle Schrödinger equation hence is not form invariant under the transformation given by (11.191). Rather, (11.193) describes a particle in an electromagnetic four-potential $\{(A^\mu)'\} = \{\partial^\mu\chi\}$! The local phase transformation thus has modified the free particle Schrödinger equation into an equation in which electromagnetic forces are present. From an observational point of view it is thus impossible to distinguish between the effects of local phase transformations and electromagnetic forces. A generalized form of phase invariance underlies the theories of the electro-weak and strong interactions in elementary particle physics.

Chapter 12

Quantum Theory of the Generalized Nonlocal Linear Response

12.1 Mean Value of the Orbital Current Density Operator in a Weak External Electromagnetic Field

When a system of charged particles is subjected to a prescribed external electromagnetic field an induced current density distribution will in general be generated in the particle system. If the external field is sufficiently weak the induced current density distribution will be related in a linear fashion to the external field, as described from different points of views, and in general terms in Chap. 10. In the present section, we shall see how a generalized linear constitutive equation of the form given in (10.79) appears from quantum mechanical considerations. In the quantum theory, the microscopic current density $\mathbf{J}(\mathbf{r}, t)$ is identified with the mean value of the particle system's current density operator $\hat{\mathbf{J}} = \sum_{\alpha} \hat{\mathbf{J}}_{\alpha}$, $\hat{\mathbf{J}}_{\alpha}$ being the current density operator of particle α . Since the initial (field unperturbed) quantum state of the particle system is not perfectly determined in general the mean value of $\hat{\mathbf{J}}$ must be calculated from $\langle \hat{\mathbf{J}} \rangle = \text{Tr}\{\hat{\rho}\hat{\mathbf{J}}\}$, cf. (11.37). The density matrix operator $\hat{\rho}$ of the system has a part which depends on the external electromagnetic field, and for weak fields this part can be determined by solving the Liouville equation iteratively.

12.1.1 Gauge Choices for the External and Induced Potentials: Interaction Hamiltonian

Under the influence of a prescribed external (ext) electromagnetic field, described by the potentials $(\mathbf{A}^{\text{ext}}, \phi^{\text{ext}})$, an induced (ind) field, given by the potentials $(\mathbf{A}^{\text{ind}}, \phi^{\text{ind}})$, is generated by the dynamical evolution of the system particles under study. In a selfconsistent manner, the charge and current densities of the particles in the system arise from the simultaneous action of the external field and the field created by the particle dynamics, i.e., from a resulting field described by the transverse and longitudinal vector potentials

$$\mathbf{A}_{\text{T}}(\mathbf{r}, t) = \mathbf{A}_{\text{T}}^{\text{ext}}(\mathbf{r}, t) + \mathbf{A}_{\text{T}}^{\text{ind}}(\mathbf{r}, t), \quad (12.1)$$

$$\mathbf{A}_L(\mathbf{r}, t) = \mathbf{A}_L^{\text{ext}}(\mathbf{r}, t) + \mathbf{A}_L^{\text{ind}}(\mathbf{r}, t), \quad (12.2)$$

and the scalar potential

$$\phi(\mathbf{r}, t) = \phi^{\text{ext}}(\mathbf{r}, t) + \phi^{\text{ind}}(\mathbf{r}, t). \quad (12.3)$$

In the presence of the external field, the nonrelativistic Hamiltonian operator of our system is in the configuration space representation given by

$$\hat{H} = \sum_{\alpha} \left\{ \frac{1}{2m_{\alpha}} [\hat{\mathbf{p}}_{\alpha} - q_{\alpha} (\mathbf{A}_T(\mathbf{r}_{\alpha}, t) + \mathbf{A}_L(\mathbf{r}_{\alpha}, t))]^2 + q_{\alpha} \phi(\mathbf{r}_{\alpha}, t) \right\}, \quad (12.4)$$

where $\hat{\mathbf{p}}_{\alpha} = -i\hbar\nabla_{\alpha}$, cf. (11.101).

It is useful for the quantum mechanical calculation of the linear response tensor (Sects. 12.2 and 12.3) to choose the Coulomb gauge for the *induced* potentials. In this gauge, the longitudinal part of the induced vector potential vanishes, so that

$$\mathbf{A}_L^{\text{ind}}(\mathbf{r}_{\alpha}, t) = \mathbf{0} \quad (12.5)$$

for all α . As shown in Sect. 9.3.1, the scalar potential (here ϕ^{ind}) then can be identified with the Coulomb potential of the charge distribution (9.55). In the Hamilton operator given in (12.4), one therefore gets

$$\sum_{\alpha} q_{\alpha} \phi^{\text{ind}}(\mathbf{r}_{\alpha}, t) = \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}|}, \quad (12.6)$$

omitting the Coulomb self-energies of the various particles, cf. (9.67) and (9.68). The self-energies play no role in the following. The right side of (12.6) may be recognized as the sum of the Coulomb interaction energies between the various pairs (α, β) of particles. In wave function space, this energy only depends on the position variables of the particles.

It is not necessary to choose the Coulomb gauge for the external potentials, although this choice has been made for the induced potentials. For the following analysis it is useful to use instead a gauge where $\phi^{\text{ext}}(\mathbf{r}, t) = 0$. Such a choice is clearly possible; see (2.12). With

$$\phi^{\text{ext}}(\mathbf{r}_{\alpha}, t) = 0 \quad (12.7)$$

for all α , the Hamilton operator in (12.4) finally takes the form

$$\hat{H} = \sum_{\alpha} \frac{1}{2m_{\alpha}} (\hat{\mathbf{p}}_{\alpha} - q_{\alpha} \mathbf{A}(\mathbf{r}_{\alpha}, t))^2 + \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}|}, \quad (12.8)$$

where

$$\mathbf{A}(\mathbf{r}_{\alpha}, t) = \mathbf{A}_T(\mathbf{r}_{\alpha}, t) + \mathbf{A}_L^{\text{ext}}(\mathbf{r}_{\alpha}, t). \quad (12.9)$$

With the gauge choices above the longitudinal part of the electric field is related to the potential (A_L^{ext}) and particle variables ($\{\mathbf{r}_\alpha\}$) as follows:

$$\mathbf{E}_L(\mathbf{r}, t) = -\frac{\partial}{\partial t} A_L^{\text{ext}}(\mathbf{r}, t) + \frac{1}{4\pi\epsilon_0} \sum_{\alpha} q_{\alpha} \frac{\mathbf{r} - \mathbf{r}_{\alpha}}{|\mathbf{r}_{\alpha} - \mathbf{r}_{\alpha}|^3}. \quad (12.10)$$

It appears from (9.44) and (9.45) that the transverse and longitudinal parts of the external vector potential in the $\phi^{\text{ext}} = 0$ -gauge satisfy the equations

$$\square A_T^{\text{ext}}(\mathbf{r}, t) = -\mu_0 \mathbf{J}_T^{\text{ext}}(\mathbf{r}, t), \quad (12.11)$$

$$\frac{\partial^2}{\partial t^2} A_L^{\text{ext}}(\mathbf{r}, t) = \frac{1}{\epsilon_0} \mathbf{J}_L^{\text{ext}}(\mathbf{r}, t). \quad (12.12)$$

For a prescribed external current density $\mathbf{J}^{\text{ext}} = \mathbf{J}_T^{\text{ext}} + \mathbf{J}_L^{\text{ext}}$ the physically acceptable explicit solutions to (12.11) and (12.12) are

$$A_T^{\text{ext}}(\mathbf{r}, t) = \mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \mathbf{J}_T^{\text{ext}}(\mathbf{r}', t') d^3 r' dt', \quad (12.13)$$

where $g(|\mathbf{r} - \mathbf{r}'|, t - t')$ is the Huygens propagator, and

$$A_L^{\text{ext}}(\mathbf{r}, t) = -(2\pi\epsilon_0)^{-1} \int_{-\infty}^{\infty} \omega^{-2} \mathbf{J}_L^{\text{ext}}(\mathbf{r}; \omega) e^{-i\omega t} d\omega. \quad (12.14)$$

For what follows it is useful to separate the Hamilton operator in (12.8) into two parts,

$$\hat{H} = \hat{H}_P + \hat{H}_I. \quad (12.15)$$

The so-called particle (P) Hamiltonian, given by

$$\hat{H}_P = \sum_{\alpha} \frac{\hat{\mathbf{p}}_{\alpha}^2}{2m_{\alpha}} + \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}|}, \quad (12.16)$$

only depends on the canonically conjugate particle operators $\{\hat{\mathbf{r}}_{\alpha} = \mathbf{r}_{\alpha}, \hat{\mathbf{p}}_{\alpha}\}$. Although $\hat{H}_P$ is called the particle Hamiltonian it is in general not an operator which coincides with the proper energy operator of the particle system (defined as the sum of the *bare* kinetic energy and mutual potential energy operators), since the operators $\{\hat{\mathbf{p}}_{\alpha}\}$ are not equal to the mechanical momentum operators $\{\hat{\boldsymbol{\pi}}_{\alpha}\}$. Even if the vectorial potential $A_{T,\alpha}^{\text{self}}$ of the particle's self-field (times q_{α}) is added to the mechanical momentum the two operator sets $\{\hat{\mathbf{p}}_{\alpha}\}$ and $\{\hat{\boldsymbol{\pi}}_{\alpha} + q_{\alpha} A_{T,\alpha}^{\text{self}}\}$ are different. The operator $\hat{H}_I$, called the interaction (*I*) Hamiltonian because it depends on both the particle operators $\{\hat{\mathbf{r}}_{\alpha}, \hat{\mathbf{p}}_{\alpha}\}$ and the electromagnetic field (through the vector potential), is conveniently divided into two pieces,

$$\hat{H}_I = \hat{H}_{I,1} + \hat{H}_{I,2}, \quad (12.17)$$

where

$$\hat{H}_{1,1} = - \sum_{\alpha} \frac{q_{\alpha}}{2m_{\alpha}} (\hat{\mathbf{p}}_{\alpha} \cdot \mathbf{A}(\mathbf{r}_{\alpha}, t) + \mathbf{A}(\mathbf{r}_{\alpha}, t) \cdot \hat{\mathbf{p}}_{\alpha}) \quad (12.18)$$

is linear in the vector potential, and

$$\hat{H}_{1,2} = \sum_{\alpha} \frac{q_{\alpha}^2}{2m_{\alpha}} \mathbf{A}(\mathbf{r}_{\alpha}, t) \cdot \mathbf{A}(\mathbf{r}_{\alpha}, t) \quad (12.19)$$

quadratic. In the *Coulomb gauge*, $\hat{H}_{1,1}$ can also be written in the form

$$\hat{H}_{1,1} = - \sum_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} \hat{\mathbf{p}}_{\alpha} \cdot \mathbf{A}(\mathbf{r}_{\alpha}, t). \quad (12.20)$$

To prove the correctness of (12.20) it is sufficient to consider a single particle (omit index α) with wave function $\Psi(\mathbf{r}, t)$ in configuration space. Thus,

$$\hat{\mathbf{p}} \cdot (\mathbf{A}\Psi) = -i\hbar \nabla \cdot (\mathbf{A}\Psi) = -i\hbar [(\nabla \cdot \mathbf{A})\Psi + \mathbf{A} \cdot \nabla \Psi] = \mathbf{A} \cdot \hat{\mathbf{p}}\Psi, \quad (12.21)$$

since $\nabla \cdot \mathbf{A} = 0$. Because Ψ is arbitrary one obtains the operator identity $\hat{\mathbf{p}} \cdot \mathbf{A} = \mathbf{A} \cdot \hat{\mathbf{p}}$ in the Coulomb gauge. This identity readily leads to the equality of the expressions in (12.18) and (12.20).

12.1.2 Iterative Solution of the Liouville Equation

For the subsequent calculation it is convenient to change the notation for the three parts of the Hamiltonian to $\hat{H}_{\text{p}} = \hat{H}_0$, $\hat{H}_{1,1} = \hat{H}_1$ and $\hat{H}_{1,2} = \hat{H}_2$, so that

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t) + \hat{H}_2(t). \quad (12.22)$$

Since $\hat{H}(t)$ depends on the vectorial potential the density matrix operator, which obeys the Liouville equation in (11.53), will also depend on $\mathbf{A}$. If the electromagnetic field is sufficiently weak it is fruitful to expand the (unknown) density matrix operator in powers of $\mathbf{A}$ that is

$$\hat{\rho}(t) = \hat{\rho}_0 + \hat{\rho}_1(t) + \hat{\rho}_2(t) + \cdots, \quad (12.23)$$

where $\hat{\rho}_i(t)$ is proportional to the i th power of $\mathbf{A}$. Since the particle Hamiltonian, $\hat{H}_0$, is time independent, so will $\hat{\rho}_0$ be. To zeroth order in $\mathbf{A}$ one thus obtains from the Liouville equation

$$0 = [\hat{H}_0, \hat{\rho}_0]. \quad (12.24)$$

Equalizing terms of first order in $\mathbf{A}$ one gets from (11.53)

$$i\hbar \frac{d}{dt} \hat{\rho}_1(t) = [\hat{H}_0, \hat{\rho}_1(t)] + [\hat{H}_1(t), \hat{\rho}_0]. \quad (12.25)$$

With a knowledge of $\hat{\rho}_0$, $\hat{\rho}_1(t)$ can be determined from this equation. For $n \geq 2$, $\hat{\rho}_n(t)$ satisfies the dynamical equation

$$i\hbar \frac{d}{dt} \hat{\rho}_n(t) = [\hat{H}_0, \hat{\rho}_n(t)] + [\hat{H}_1(t), \hat{\rho}_{n-1}] + [\hat{H}_2(t), \hat{\rho}_{n-2}(t)], \quad (12.26)$$

and with a knowledge of $\hat{\rho}_{n-2}(t)$ and $\hat{\rho}_{n-1}(t)$, $\hat{\rho}_n(t)$ can be obtained from this equation. Given $\hat{\rho}_0$, the iterative solution of the Liouville equation allows one to obtain the density matrix operator in form of a power expansion in the vector potential given in (12.9). To determine the linear (in $\mathbf{A}$) part of the current density induced by the external field only $\hat{\rho}_1(t)$ is needed, as we shall realize below.

12.1.3 Linearized Orbital Current Density

In configuration space the orbital current density operator of our particle system is given by (with $\hat{\mathbf{p}}_\alpha = -i\hbar \nabla_\alpha$)

$$\hat{\mathbf{j}}(\mathbf{r}, t) = \sum_\alpha \frac{q_\alpha}{2m_\alpha} [\delta(\mathbf{r} - \mathbf{r}_\alpha) (\hat{\mathbf{p}}_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t)) + (\hat{\mathbf{p}}_\alpha - q_\alpha \mathbf{A}(\mathbf{r}_\alpha, t)) \delta(\mathbf{r} - \mathbf{r}_\alpha)], \quad (12.27)$$

and with the gauge choice in Sect. 12.1.2, $\mathbf{A} = \mathbf{A}_T + \mathbf{A}_L^{\text{ext}}$. That $\hat{\mathbf{j}}$ is given by the expression in (12.27) follows from the fact that the particle current density operator is a one-body operator (given for particle $\alpha = q$ in (11.140), with $\hat{\boldsymbol{\pi}}$ taken from (11.135)). The current density operator now is separated into two parts,

$$\hat{\mathbf{j}} = \hat{\mathbf{j}}_0 + \hat{\mathbf{j}}_1, \quad (12.28)$$

where

$$\hat{\mathbf{j}}_0 = \sum_\alpha \frac{q_\alpha}{2m_\alpha} (\delta(\mathbf{r} - \mathbf{r}_\alpha) \hat{\mathbf{p}}_\alpha + \hat{\mathbf{p}}_\alpha \delta(\mathbf{r} - \mathbf{r}_\alpha)) \quad (12.29)$$

is independent of the vector potential, but gauge dependent (cf. the remarks in Sect. 11.6.1), and

$$\hat{\mathbf{j}}_1 = - \sum_\alpha \frac{q_\alpha^2}{m_\alpha} \mathbf{A}(\mathbf{r}_\alpha, t) \delta(\mathbf{r} - \mathbf{r}_\alpha) \quad (12.30)$$

is linear in the vector potential, and thus manifestly gauge dependent.

The mean value of the current density operator, given in configuration space by (see (11.37))

$$\mathbf{J}(\mathbf{r}, t) \equiv \langle \hat{\mathbf{j}} \rangle(t) = Tr\{\hat{\rho}(t) \hat{\mathbf{j}}(t)\} \quad (12.31)$$

can be expressed in a power series of $\mathbf{A}$ by insertion of (12.23) and (12.28). Thus,

$$\mathbf{J}(\mathbf{r}, t) = Tr\{\hat{\rho}_0 \hat{\mathbf{j}}_0\} + \sum_{n=0}^{\infty} \left[Tr\{\hat{\rho}_n(t) \hat{\mathbf{j}}_1(t)\} + Tr\{\hat{\rho}_{n+1}(t) \hat{\mathbf{j}}_0\} \right]. \quad (12.32)$$

If it is assumed that the mean current density is zero in absence of the external field one has

$$Tr\{\hat{\rho}_0 \hat{\mathbf{j}}_0\} = \mathbf{0}, \quad (12.33)$$

and, if hereafter only the part of the current density which is linear in the vector potential is retained, (12.32) gives

$$\mathbf{J}(\mathbf{r}, t) = Tr\{\hat{\rho}_0 \hat{\mathbf{j}}_1(t)\} + Tr\{\hat{\rho}_1(t) \hat{\mathbf{j}}_0\}. \quad (12.34)$$

Starting from (12.25) and (12.34) the generalized linear and nonlocal response tensor can be determined quantum mechanically, in principle at least. The time independence of $\hat{\rho}_0$ and $\hat{\mathbf{j}}_0$ implies that the response tensor exhibits translational invariance in time, i.e., $\mathbf{S}(\mathbf{r}, \mathbf{r}', t, t') = \mathbf{S}(\mathbf{r}, \mathbf{r}', t - t')$. In the frequency domain $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ therefore can be calculated from the two algebraic equations

$$\mathbf{J}(\mathbf{r}; \omega) = Tr\{\hat{\rho}_0 \hat{\mathbf{j}}_1(\omega)\} + Tr\{\hat{\rho}_1(\omega) \hat{\mathbf{j}}_0\}, \quad (12.35)$$

$$\hbar \omega \hat{\rho}_1(\omega) = [\hat{H}_0, \hat{\rho}_1(\omega)] + [\hat{H}_1(\omega), \hat{\rho}_0]. \quad (12.36)$$

The reader may note that the Hamiltonian $\hat{H}_{l,2}$ (12.19) does not enter the linear response theory. With the gauge choices of Sect. 12.1.1, the Fourier transform of $\hat{H}_{l,1}(t) \equiv \hat{H}_1(t)$ is

$$\hat{H}_1(\omega) = - \sum_{\alpha} \frac{q_{\alpha}}{2m_{\alpha}} (\hat{\mathbf{p}}_{\alpha} \cdot \mathbf{A}(\mathbf{r}_{\alpha}; \omega) + \mathbf{A}(\mathbf{r}_{\alpha}; \omega) \cdot \hat{\mathbf{p}}_{\alpha}), \quad (12.37)$$

with $\mathbf{A}(\mathbf{r}_{\alpha}; \omega) = \mathbf{A}_T(\mathbf{r}_{\alpha}; \omega) + \mathbf{A}_L^{\text{ext}}(\mathbf{r}_{\alpha}; \omega)$.

12.1.4 Calculation of the Mean Current Density in the $\hat{H}_0$ -Basis

Independent of which basis is used, the mean value of the observable current density operator, $\langle \hat{\mathbf{j}} \rangle(t)$, must of course be the same. This is guaranteed by the fact that the trace of an operator (here $\hat{\rho} \hat{\mathbf{j}}$) is the same in every basis representation [164]. The form of (12.36) (and (12.25)) indicates that it will be fruitful to use as basis a complete set of many-body eigenfunctions for the field unperturbed Hamiltonian, $\hat{H}_0$. In general, the eigenfunctions of $\hat{H}_0$ will be degenerate, and various basis sets therefore can be chosen. For what follows the specific choice is not relevant. In the Dirac notation, to be used below, the orthonormalized many-body eigenkets of $\hat{H}_0$ are denoted by $|I\rangle$ (or $|J\rangle$) and the related eigenenergies by E_I (or E_J). The eigenvalue equation for $\hat{H}_0 = \hat{H}_0(\{\hat{\mathbf{r}}_{\alpha}\}, \{\hat{\mathbf{p}}_{\alpha}\})$ hence reads

$$\hat{H}_0|I\rangle = E_I|I\rangle. \quad (12.38)$$

Since $\hat{H}_0$ and $\hat{\rho}_0$ commute (12.24), the states $\hat{\rho}_0|I\rangle$ are also eigenstates for $\hat{H}_0$ with eigenvalues E_I , i.e.,

$$\hat{H}_0(\hat{\rho}_0|I\rangle) = E_I(\hat{\rho}_0|I\rangle). \quad (12.39)$$

Let us now assume that the particle system is in thermodynamic equilibrium in the absence of external fields. Then,

$$\hat{\rho}_0|I\rangle = P_I|I\rangle, \quad (12.40)$$

where P_I is the probability for the many-body state $|I\rangle$ being occupied. In thermodynamic equilibrium the many-body density matrix operator is given by

$$\hat{\rho}_0 = \frac{\exp(-\beta\hat{H}_0)}{\text{Tr}\{\exp(-\beta\hat{H}_0)\}}, \quad (12.41)$$

where $\beta = (k_B T)^{-1}$, k_B being Boltzmann's constant and T the absolute temperature. The denominator in (12.41) ensures that $\text{Tr}\{\hat{\rho}_0\} = 1$, as required (see (11.39)).

By inserting the unit operator, written via the closure theorem as

$$\hat{1} = \sum_J |J\rangle\langle J|, \quad (12.42)$$

inbetween the density matrix and current density operators appearing in the two traces of (12.35) one obtains

$$\mathbf{J}(\mathbf{r}; \omega) = \sum_{I,J} \langle I|\hat{\rho}_0|J\rangle \langle J|\hat{\mathbf{j}}_1(\omega)|I\rangle + \sum_{I,J} \langle I|\hat{\rho}_1(\omega)|J\rangle \langle J|\hat{\mathbf{j}}_0|I\rangle. \quad (12.43)$$

The first double sum in (12.43) can be reduced to a single sum utilizing (12.40) and the orthonormality condition $\langle I|J\rangle = \delta_{IJ}$, as one readily realizes:

$$\langle I|\hat{\rho}_0|J\rangle = P_J \langle I|J\rangle = P_I \delta_{IJ}. \quad (12.44)$$

In the second double sum, the matrix elements of $\hat{\rho}_1(\omega)$ can be calculated via (12.36). The IJ th matrix element hence satisfies the equation

$$\hbar\omega \langle I|\hat{\rho}_1(\omega)|J\rangle = \langle I|\hat{H}_0\hat{\rho}_1(\omega) - \hat{\rho}_1(\omega)\hat{H}_0|J\rangle + \langle I|\hat{H}_1(\omega)\hat{\rho}_0 - \hat{\rho}_0\hat{H}_1(\omega)|J\rangle, \quad (12.45)$$

and since $\hat{H}_0$ and $\hat{\rho}_0$ are Hermitian ($\hat{H}_0$ is manifestly Hermitian, and the eigenvalues of $\hat{\rho}_0$ are real), use of (12.38) and (12.40), and their associated bra relations, give

$$\langle I|\hat{\rho}_1(\omega)|J\rangle = \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \langle I|\hat{H}_1(\omega)|J\rangle. \quad (12.46)$$

By means of (12.44) and (12.46), the current density in (12.43) can be written in the form

$$\mathbf{J}(\mathbf{r}; \omega) = \sum_I P_I \langle I | \hat{\mathbf{j}}_1(\omega) | I \rangle + \sum_{I,J} \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \langle I | \hat{H}_1(\omega) | J \rangle \langle J | \hat{\mathbf{j}}_0 | I \rangle. \quad (12.47)$$

It is clear the the genuine diamagnetic part of the current density is contained in the single sum of (12.47), and given via those terms in $\hat{\mathbf{j}}_1(\omega)$ (12.30) that contain the transverse vector potential A_T , cf. (12.9) and the discussion in Sect. 11.5.2.

12.2 The Nonlocal Linear Response Tensor

In the following we shall assume that all the particles which participate in an important fashion to the dynamic electromagnetic response are electrons ((rest)mass m , and charge $-e$). A generalization to situations where also the motions of nuclei are of importance can be made.

12.2.1 One-Electron Approximation

From a calculational (numerical) point of view it is most often necessary to approximate the many-body particle Hamiltonian in (12.16) by some sort of single-particle Hamiltonian, and over the years much effort has been devoted to attempts to construct accurate Hamiltonians for single electrons. For the present purpose it is not necessary to discuss the various kinds of single-particle potentials (Hartree, Hartree-Fock, Kohn-Sham, [118, 207]) which have been used in the literature. For the one-electron Hamiltonian $\hat{H}_0$ we denote the orthonormalized eigenkets by $|i\rangle$ (or $|j\rangle$) and the associated eigenenergies by ϵ_i (or ϵ_j). The various single-particle states are characterized by a triple set of spatial quantum numbers, and the subscript i (or j) therefore stands for three numbers. In the $\{|\mathbf{r}\rangle\}$ representation the eigenvalue equation for the single-electron particle Hamiltonian thus is

$$\hat{H}_0 \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}), \quad (12.48)$$

where $\hat{H}_0$ now is the particle Hamiltonian in this representation, and $\psi_i(\mathbf{r}) = \langle \mathbf{r} | i \rangle$ is the time independent wave function belonging to the eigenstate i of energy ϵ_i . In thermodynamic equilibrium, the field unperturbed single-particle density matrix given by

$$\hat{\rho}_0 = \sum_i f_i |i\rangle \langle i|, \quad (12.49)$$

where f_i is the properly normalized (see below) probability that the single-particle energy eigenstate $|i\rangle$ is occupied, satisfies in configuration space [$\hat{\rho}_0 \equiv \langle \mathbf{r} | \hat{\rho}_0 | \mathbf{r}' \rangle$ $\delta(\mathbf{r} - \mathbf{r}')$] the equation

$$\hat{\rho}_0 \psi_i(\mathbf{r}) = f_i \psi_i(\mathbf{r}). \quad (12.50)$$

In thermal equilibrium, f_i is for electrons the Fermi–Dirac distribution function (factor)

$$f_i = \{\exp[(\epsilon_i - \mu)/(k_B T)] + 1\}^{-1}, \quad (12.51)$$

where μ is the chemical potential. In the present “spinless” calculation, where the summation over the electron’s spin states just appears as a factor of two in the final response tensor, the chemical potential $\mu = \mu(T)$ has such a value that the Fermi–Dirac distribution factor is normalized to half the number of electrons in the system under study. If we temporarily denote the one-electron coordinate and momentum operators by $\hat{\mathbf{r}}_e = \mathbf{r}_e$ and $\hat{\mathbf{p}}_e = -i\hbar\nabla_e$, respectively, the (linearized) interaction Hamiltonian is given by

$$\hat{H}_1(\omega) = \frac{e}{2m} (\hat{\mathbf{p}}_e \cdot \mathbf{A}(\mathbf{r}_e; \omega) + \mathbf{A}(\mathbf{r}_e; \omega) \cdot \hat{\mathbf{p}}_e) \quad (12.52)$$

in the space–frequency domain, and the two parts of the current density operator by

$$\hat{\mathbf{j}}_0(\mathbf{r}; \omega) = -\frac{e}{2m} (\delta(\mathbf{r} - \mathbf{r}_e) \hat{\mathbf{p}}_e + \hat{\mathbf{p}}_e \delta(\mathbf{r} - \mathbf{r}_e)), \quad (12.53)$$

and

$$\hat{\mathbf{j}}_1(\mathbf{r}; \omega) = -\frac{e^2}{m} \mathbf{A}(\mathbf{r}_e; \omega) \delta(\mathbf{r} - \mathbf{r}_e). \quad (12.54)$$

In the one-electron approximation the contribution to the current density from the single sum in (12.47) becomes

$$\begin{aligned} 2 \sum_i f_i \langle i | \hat{\mathbf{j}}_1(\omega) | i \rangle &= -\frac{2e^2}{m} \sum_i f_i \int_{-\infty}^{\infty} \psi_i^*(\mathbf{r}_e) \mathbf{A}(\mathbf{r}_e; \omega) \delta(\mathbf{r} - \mathbf{r}_e) \psi_i(\mathbf{r}_e) d^3 r_e \\ &= -\frac{2e^2}{m} \mathbf{A}(\mathbf{r}; \omega) \sum_i f_i |\psi_i(\mathbf{r})|^2. \end{aligned} \quad (12.55)$$

The factor of two in front of the summation sign stems from the spin degeneracy. Since the quantity

$$N_0(\mathbf{r}) = 2 \sum_i f_i |\psi_i(\mathbf{r})|^2 \quad (12.56)$$

is just the electron density at $\mathbf{r}$, one can conclude that

$$2 \sum_i f_i \langle i | \hat{\mathbf{j}}_1(\omega) | i \rangle = -\frac{e^2}{m} N_0(\mathbf{r}) \mathbf{A}(\mathbf{r}; \omega). \quad (12.57)$$

To evaluate the contribution to $\mathbf{J}(\mathbf{r}; \omega)$ from the double sum in (12.47) we first calculate the two matrix elements $\langle j | \hat{\mathbf{j}}_0 | i \rangle$ and $\langle i | \hat{H}_1(\omega) | j \rangle$. Since $\hat{\mathbf{p}}_e$ is Hermitian, we obtain

$$\langle j | \hat{\mathbf{j}}_0 | i \rangle = -\frac{e}{2m} \int_{-\infty}^{\infty} \left[\psi_j^*(\mathbf{r}_e) \hat{\mathbf{p}}_e \psi_i(\mathbf{r}_e) + (\hat{\mathbf{p}}_e \psi_j(\mathbf{r}_e))^* \psi_i(\mathbf{r}_e) \right] \delta(\mathbf{r} - \mathbf{r}_e) d^3 r_e, \quad (12.58)$$

and hence

$$\langle j | \hat{\mathbf{j}}_0 | i \rangle = -\frac{e\hbar}{2mi} (\psi_j^*(\mathbf{r}) \nabla \psi_i(\mathbf{r}) - \psi_i(\mathbf{r}) \nabla \psi_j^*(\mathbf{r})). \quad (12.59)$$

The result in (12.59) relates closely to the transition current density discussed in Sect. 11.5.3. If one in (11.134) makes the division

$$\mathbf{j}_{i \rightarrow j}(\mathbf{r}, t) = \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) + \mathbf{j}_{i \rightarrow j}^1(\mathbf{r}, t), \quad (12.60)$$

where

$$\mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) = \frac{q\hbar}{2mi} (u_j^*(\mathbf{r}) \nabla u_i(\mathbf{r}) - u_i(\mathbf{r}) \nabla u_j^*(\mathbf{r})), \quad (12.61)$$

and

$$\mathbf{j}_{i \rightarrow j}^1(\mathbf{r}, t) = -\frac{q^2}{m} \mathbf{A}(\mathbf{r}, t) u_i(\mathbf{r}) u_j^*(\mathbf{r}), \quad (12.62)$$

the reader realizes that the right-hand side of (12.59) equals the vector potential independent part of the transition current density for the electron ($q = -e$), the transition being between energy eigenstates. Thus,

$$\langle j | \hat{\mathbf{j}}_0 | i \rangle = \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}). \quad (12.63)$$

Utilizing again that $\hat{\mathbf{p}}_e = \hat{\mathbf{p}}_e^\dagger$, it is not difficult to show that

$$\langle i | \hat{H}_1(\omega) | j \rangle = \frac{e\hbar}{2mi} \int_{-\infty}^{\infty} (\psi_i^*(\mathbf{r}_e) \nabla \psi_j(\mathbf{r}_e) - \psi_j(\mathbf{r}_e) \nabla \psi_i^*(\mathbf{r}_e)) \cdot \mathbf{A}(\mathbf{r}_e; \omega) d^3 r_e. \quad (12.64)$$

If the vectorial integration variable is changed from $\mathbf{r}_e$ to $\mathbf{r}'$, and (12.61) is used, one gets

$$\langle i | \hat{H}_1(\omega) | j \rangle = - \int_{-\infty}^{\infty} \mathbf{j}_{j \rightarrow i}^0(\mathbf{r}') \cdot \mathbf{A}(\mathbf{r}'; \omega) d^3 r'. \quad (12.65)$$

The results in (12.63) and (12.65) finally lead to the following expression for the double sum in (12.47) in the one-electron approximation:

$$\begin{aligned} & 2 \sum_{i,j} \frac{f_j - f_i}{\hbar\omega + \epsilon_j - \epsilon_i} \langle i | \hat{H}_1(\omega) | j \rangle \langle j | \hat{\mathbf{j}}_0 | i \rangle \\ &= -2 \sum_{i,j} \frac{f_j - f_i}{\hbar\omega + \epsilon_j - \epsilon_i} \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) \int_{-\infty}^{\infty} \mathbf{j}_{j \rightarrow i}^0(\mathbf{r}') \cdot \mathbf{A}(\mathbf{r}'; \omega) d^3 r'. \end{aligned} \quad (12.66)$$

In the framework of the one-electron theory, the linearized current density in (12.47) consists of the sum of the contributions in (12.57) and (12.66), with the vector potential given by the Fourier (ω) transform of (12.9). This potential can be replaced by

$$\mathbf{A}_T + \mathbf{A}_L^{\text{ext}} = (i\omega)^{-1}(\mathbf{E}_T + \mathbf{E}_L^{\text{ext}}) \quad (12.67)$$

since $\mathbf{A}_T$ is gauge independent, and $\phi^{\text{ext}} = 0$ (cf. (12.10)). In the view of this connection, the one-electron quantum theory leads to a linear and nonlocal constitutive equation of the form

$$\mathbf{J}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) \cdot (\mathbf{E}_T(\mathbf{r}'; \omega) + \mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega)) d^3r' \quad (12.68)$$

with a generalized linear response tensor given by

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{2i}{\omega} \sum_{i,j} \frac{f_j - f_i}{\hbar\omega + \epsilon_j - \epsilon_i} \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) \mathbf{j}_{j \rightarrow i}^0(\mathbf{r}') + \frac{ie^2}{m\omega} N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \mathbf{U}. \quad (12.69)$$

At this point the reader may note that (12.68) has precisely the form (10.79) would take in the space–frequency domain for media exhibiting translational invariance in time [$\mathbf{S}(\mathbf{r}, \mathbf{r}', t, t') \Rightarrow \mathbf{S}(\mathbf{r}, \mathbf{r}', t - t')$]. The last term in (12.69) relates the current density and the appropriate electric field in a spatially local manner, and the term is usually called the diamagnetic response tensor. The remaining part of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ is called the paramagnetic response tensor. This part relates the current density to the electric field in a spatially nonlocal manner. The range of this nonlocality is of the order of the extension of the energy orbitals $\psi_i(\mathbf{r})$, cf. (12.59) and (12.63).

The paramagnetic part of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ consists of a sum of weighted tensor products $\mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) \mathbf{j}_{j \rightarrow i}^0(\mathbf{r}')$ in which the first vector is a function of $\mathbf{r}$, the second of $\mathbf{r}'$. As we shall realize in Sect. 12.4, it is possible to write also the diamagnetic term in such a form. The tensor product structure allows one to establish a rigorous microscopic theory of local-field effects in mesoscopic electrodynamics and near-field optics (Chap. 13).

12.2.2 Many-Body Approach

In a many-electron calculation of the generalized response tensor, one obtains for $\mathbf{S}(\mathbf{r}, \mathbf{r}; \omega)$ an expression which *formal structure* is completely identical to the one given in (12.69). To prove this, let us first introduce a notation for the many-body wave functions in configuration space. If the state vector

$$|\{\mathbf{r}_\alpha\}\rangle \equiv |\mathbf{r}_1\rangle |\mathbf{r}_2\rangle \cdots |\mathbf{r}_\alpha\rangle \cdots \quad (12.70)$$

describes the quantum state in which the system particles (electrons) definitely are located at the positions $\mathbf{r}_1, \mathbf{r}_2 \dots \mathbf{r}_\alpha \dots$, the many-electron wave function representing in configuration space the many-body energy eigenstate $|I\rangle$ is

$$\langle \{\mathbf{r}_\alpha\} | I \rangle = \Psi_I(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_\alpha, \dots), \quad (12.71)$$

cf. the description in Sect. 11.3. To determine the contribution to the current density $\mathbf{J}(\mathbf{r}; \omega)$ from the single sum in (12.47) we first calculate the matrix element $\langle I | \hat{\mathbf{j}}_1(\omega) | I \rangle$. Thus,

$$\begin{aligned} \langle I | \hat{\mathbf{j}}_1(\omega) | I \rangle &= -\frac{e^2}{m} \sum_{\alpha} \int_{-\infty}^{\infty} |\Psi_I|^2 \delta(\mathbf{r} - \mathbf{r}_{\alpha}) \mathbf{A}(\mathbf{r}_{\alpha}; \omega) \prod_{\beta} d^3 r_{\beta} \\ &= -\frac{e^2}{m} \mathbf{A}(\mathbf{r}; \omega) \sum_{\alpha} \int_{-\infty}^{\infty} |\Psi_I|^2 \delta(\mathbf{r} - \mathbf{r}_{\alpha}) \prod_{\beta} d^3 r_{\beta}, \end{aligned} \quad (12.72)$$

in a notation where the summation $\sum_{\alpha}$ and product $\prod_{\beta}$ run over all the electron coordinates $\{\mathbf{r}_{\alpha}\}(\{\mathbf{r}_{\beta}\})$. If with certainty the electron system is in the quantum state Ψ_I the quantity

$$N_{0,I}(\mathbf{r}) = \sum_{\alpha} \int_{-\infty}^{\infty} |\Psi_I|^2 \delta(\mathbf{r} - \mathbf{r}_{\alpha}) \prod_{\beta} d^3 r_{\beta} \quad (12.73)$$

is just the electron density at $\mathbf{r}$ in the field unperturbed state. The many-body state Ψ_I is, however, only occupied with a probability P_I (normalized here to unity), and

$$N_0(\mathbf{r}) = \sum_I P_I N_{0,I}(\mathbf{r}) \quad (12.74)$$

therefore gives the proper electron density at $\mathbf{r}$ in the case of thermal equilibrium. Altogether, one hence obtains the result

$$\sum_I P_I \langle I | \hat{\mathbf{j}}_1(\omega) | I \rangle = -\frac{e^2}{m} N_0(\mathbf{r}) \mathbf{A}(\mathbf{r}; \omega) \quad (12.75)$$

for the first part of (12.47). A generalization of the one-electron current density $\mathbf{j}_{i \rightarrow j}^0(\mathbf{r})$ given in (12.61) to the many electron case shows that the transition current density from state A to state B is given by

$$\mathbf{J}_{A \rightarrow B}^0(\mathbf{r}) = -\frac{e\hbar}{2mi} \sum_{\alpha} \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}_{\alpha}) [\Psi_B^* \nabla_{\alpha} \Psi_A - \Psi_A \nabla_{\alpha} \Psi_B^*] \prod_{\beta} d^3 r_{\beta} \quad (12.76)$$

in the absence of the vector potential. Now, the reader may convince herself that the two matrix elements appearing in the double sum of (12.47) can be expressed in

terms of $\mathbf{J}_{A \rightarrow B}^0(\mathbf{r})$ as follows:

$$\langle J | \hat{\mathbf{j}}_0 | I \rangle = \mathbf{J}_{I \rightarrow J}^0(\mathbf{r}), \quad (12.77)$$

$$\langle I | \hat{H}_1(\omega) | J \rangle = - \int_{-\infty}^{\infty} \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}') \cdot \mathbf{A}(\mathbf{r}'; \omega) d^3 r'. \quad (12.78)$$

A combination of (12.9), (12.47), (12.67), (12.75), (12.77), and (12.78) again leads to a constitutive relation of the form given in (12.68), and now with a generalized many-electron linear and nonlocal response tensor

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\omega} \sum_{I, J} \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \mathbf{J}_{I \rightarrow J}^0(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}') + \frac{ie^2}{m\omega} N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \mathbf{U}. \quad (12.79)$$

The formal structures of the many-body (12.79) and single-body (12.69) response tensors thus are identical, remembering that spin degeneracy does not occur in general in the many-body case [$2f_i(2f_j) \rightarrow P_I(P_J)$]. In the following, I shall name the first (spatially nonlocal) part of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ the paramagnetic part, and the second (spatially local) part, the diamagnetic part, cf. the discussion in Sect. 11.5.2.

12.3 Tensor Product Structure of the Orbital Response Tensor

It appears from (12.79) that the para- and diamagnetic parts of the many-body response tensor both diverge when the frequency goes to zero. From a physical point of view only the sum of the two parts is of importance, and below we shall prove that the sum does not diverge for $\omega \rightarrow 0$. The proof is established by rewriting the spatially local diamagnetic part of $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ as a weighted double sum of *nonlocal* tensor products $\mathbf{J}_{I \rightarrow J}^0(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}')$. Addition of the para- and diamagnetic contributions altogether leads to a tensor product structure for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ which is of great importance for our understanding and the calculation of local-field phenomena in near-field electrodynamics; see Chap. 13. Irreversible damping processes are not included in (12.79), and the manner in which such processes affect the (low-frequency) behavior of the generalized response tensor is briefly discussed in Sect. 12.5.

In order to rewrite the diamagnetic contribution to $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ in the form indicated above, we shall make use of two important commutator relations, namely,

$$[\hat{H}_0, \hat{n}(\mathbf{r})] = \frac{\hbar}{ie} \nabla \cdot \hat{\mathbf{j}}_0(\mathbf{r}), \quad (12.80)$$

and

$$[[\hat{H}_0, \hat{n}(\mathbf{r})], \hat{n}(\mathbf{r}')] = -\frac{\hbar^2}{m} \nabla \cdot \nabla' (\delta(\mathbf{r} - \mathbf{r}') \hat{n}(\mathbf{r})), \quad (12.81)$$

where

$$\hat{n}(\mathbf{r}) = \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}) \quad (12.82)$$

is the number operator for the electron system. To prove the commutator relation in (12.80), we note that

$$[\hat{H}_0, \hat{n}(\mathbf{r})] = \left[\frac{1}{2m} \sum_{\beta} \hat{\mathbf{p}}_{\beta}^2, \sum_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}) \right] = \frac{1}{2m} \sum_{\alpha} [\hat{\mathbf{p}}_{\alpha}^2, \delta(\mathbf{r} - \mathbf{r}_{\alpha})]. \quad (12.83)$$

The first equality follows because the Coulomb interaction energy between different pairs of particles only depends on the position coordinates (use (11.96)), and the second equality is a consequence of (11.97). Since $\hat{\mathbf{p}}_{\alpha} \delta = \delta \hat{\mathbf{p}}_{\alpha} + \{\hat{\mathbf{p}}_{\alpha} \delta\}$, and $\hat{\mathbf{p}}_{\alpha} \cdot (\delta \hat{\mathbf{p}}_{\alpha}) = \{\hat{\mathbf{p}}_{\alpha} \delta\} \cdot \hat{\mathbf{p}}_{\alpha} + \delta \hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{p}}_{\alpha}$, in a notation where $\{\hat{\mathbf{p}}_{\alpha} \delta\}$ means that $\hat{\mathbf{p}}_{\alpha} = -i\hbar \nabla_{\alpha}$ only acts on δ , one obtains [with $\hat{\mathbf{p}}_{\alpha}^2 \equiv \hat{\mathbf{p}}_{\alpha}^2$]

$$\begin{aligned} [\hat{\mathbf{p}}_{\alpha}^2, \delta] &= \hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{p}}_{\alpha} \delta - \delta \hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{p}}_{\alpha} = \hat{\mathbf{p}}_{\alpha} \cdot \{\hat{\mathbf{p}}_{\alpha} \delta\} + \{\hat{\mathbf{p}}_{\alpha} \delta\} \cdot \hat{\mathbf{p}}_{\alpha} \\ &= -\hat{\mathbf{p}}_{\alpha} \cdot \{\hat{\mathbf{p}} \delta\} - \{\hat{\mathbf{p}} \delta\} \cdot \hat{\mathbf{p}}_{\alpha} = -\hat{\mathbf{p}} \cdot (\hat{\mathbf{p}}_{\alpha} \delta + \delta \hat{\mathbf{p}}_{\alpha}), \end{aligned} \quad (12.84)$$

since, with $\hat{\mathbf{p}} = -i\hbar \nabla$, $\{\hat{\mathbf{p}}_{\alpha} \delta\} = -\{\hat{\mathbf{p}} \delta\} = -\hat{\mathbf{p}} \delta$. The last equality follows from the fact that the many-body wave function following $\{\dots\}$ only depends on the $\{\mathbf{r}_{\alpha}\}$ coordinates. With the help of (12.84), one obtains

$$[\hat{H}_0, \hat{n}(\mathbf{r})] = \frac{\hbar}{ie} \nabla \cdot \left[-\frac{e}{2m} \sum_{\alpha} (\hat{\mathbf{p}}_{\alpha} \delta + \delta \hat{\mathbf{p}}_{\alpha}) \right], \quad (12.85)$$

and since the quantity inside the $[\dots]$ -bracket, is just $\hat{\mathbf{j}}_0(\mathbf{r})$ (see (12.29)), (12.80) has been proven. To determine the double commutator

$$[[\hat{H}_0, \hat{n}(\mathbf{r})], \hat{n}(\mathbf{r}')] = \frac{1}{2m} \sum_{\alpha} [[\hat{\mathbf{p}}_{\alpha}^2, \delta], \delta'], \quad (12.86)$$

where $\delta = \delta(\mathbf{r} - \mathbf{r}_{\alpha})$ and $\delta' = \delta(\mathbf{r}' - \mathbf{r}_{\alpha})$, we begin with

$$\begin{aligned} [[\hat{\mathbf{p}}_{\alpha}^2, \delta], \delta'] &= i\hbar \nabla \cdot (\delta \hat{\mathbf{p}}_{\alpha} \delta' + \hat{\mathbf{p}}_{\alpha} \delta \delta' - \delta' \delta \hat{\mathbf{p}}_{\alpha} - \delta' \hat{\mathbf{p}}_{\alpha} \delta) \\ &= i\hbar \nabla \cdot (\delta \hat{\mathbf{p}}_{\alpha} \delta' + \{\hat{\mathbf{p}}_{\alpha} \delta\} \delta' + \delta \{\hat{\mathbf{p}}_{\alpha} \delta'\} - \delta' \hat{\mathbf{p}}_{\alpha} \delta) \\ &= 2i\hbar \nabla \cdot (\delta \{\hat{\mathbf{p}}_{\alpha} \delta'\}). \end{aligned} \quad (12.87)$$

Since $\hat{\mathbf{p}}_{\alpha} \delta' = i\hbar \nabla' \delta'$ we next obtain

$$\begin{aligned} [[\hat{\mathbf{p}}_{\alpha}^2, \delta], \delta'] &= -2\hbar^2 \nabla \cdot \nabla' (\delta(\mathbf{r} - \mathbf{r}_{\alpha}) \delta(\mathbf{r}' - \mathbf{r}_{\alpha})) \\ &= -2\hbar^2 \nabla \cdot \nabla' (\delta(\mathbf{r} - \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}_{\alpha})). \end{aligned} \quad (12.88)$$

A summation of (12.88) over α finally leads to the double commutator relation in (12.81), q.e.d. A comparison of the right side of (12.81) with the form of the diamagnetic part of (12.79), and the fact that

$$Tr\{\hat{\rho}_0 \hat{n}(\mathbf{r})\} = \sum_I P_I \langle I | \hat{n}(\mathbf{r}) | I \rangle = \sum_I P_I N_{0,I}(\mathbf{r}) = N_0(\mathbf{r}), \quad (12.89)$$

indicate that one takes the trace of the product of the double commutator and $\hat{\rho}_0$. By utilizing the relation

$$\langle K | [\hat{H}_0, \hat{n}(\mathbf{r})] | I \rangle = (E_K - E_I) \langle K | \hat{n}(\mathbf{r}) | I \rangle, \quad (12.90)$$

and an analogous one with the replacements $K \rightarrow I$ and $I \rightarrow J$, one obtains with the help of the closure theorem (12.42)

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \left[[\hat{H}_0, \hat{n}(\mathbf{r})], \hat{n}(\mathbf{r}') \right] \right\} \\ = \sum_{I,J,K} \langle J | \hat{\rho}_0 | K \rangle \left[(E_K - E_I) \langle K | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle \right. \\ \left. - (E_I - E_J) \langle K | \hat{n}(\mathbf{r}') | I \rangle \langle I | \hat{n}(\mathbf{r}) | J \rangle \right]. \end{aligned} \quad (12.91)$$

By means of (12.44) the triple sum is reduced to a double sum:

$$\begin{aligned} Tr \left\{ \hat{\rho}_0 \left[[\hat{H}_0, \hat{n}(\mathbf{r})], \hat{n}(\mathbf{r}') \right] \right\} \\ = \sum_{I,J} P_J \left[(E_J - E_I) \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle \right. \\ \left. - (E_I - E_J) \langle J | \hat{n}(\mathbf{r}') | I \rangle \langle I | \hat{n}(\mathbf{r}) | J \rangle \right] \\ = \sum_{I,J} (P_J - P_I) (E_J - E_I) \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle. \end{aligned} \quad (12.92)$$

The last equality in (12.92) is obtained by the interchange $\langle J | \hat{n}(\mathbf{r}') | I \rangle \langle I | \hat{n}(\mathbf{r}) | J \rangle = \langle I | \hat{n}(\mathbf{r}) | J \rangle \langle J | \hat{n}(\mathbf{r}') | I \rangle$, followed by the dummy variable substitutions $I \rightarrow J$ and $J \rightarrow I$ in the term in (12.92) which contains this product of matrix elements. Together, (12.81), (12.89), and (12.92) give the important result

$$\begin{aligned} \sum_{I,J} (P_I - P_J) (E_I - E_J) \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle \\ = -\frac{\hbar^2}{m} \nabla' \cdot \nabla (N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}')). \end{aligned} \quad (12.93)$$

By taking the J Ith matrix element on the two sides of (12.80) one obtains

$$(E_J - E_I) \langle J | \hat{n}(\mathbf{r}) | I \rangle = \frac{\hbar}{ie} \nabla \cdot \langle J | \hat{\mathbf{j}}_0(\mathbf{r}) | I \rangle. \quad (12.94)$$

The relation in (12.94) plus a similar one for the matrix element of $\hat{n}(\mathbf{r}')$ allow one to replace the matrix elements of the number operators in (12.93) with matrix elements of the current density operators. Hence,

$$\begin{aligned} \nabla' \nabla : & \left[-\frac{m}{e^2} \sum_{I \neq J} \frac{P_I - P_J}{E_I - E_J} \langle J | \hat{\mathbf{j}}_0(\mathbf{r}) | I \rangle \langle I | \hat{\mathbf{j}}_0(\mathbf{r}') | J \rangle \right] \\ & = \nabla' \cdot \nabla (N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}')), \end{aligned} \quad (12.95)$$

where, as indicated, the double sum does not include terms with $I = J$. The tensor relation

$$\nabla' \cdot \nabla A = \nabla' \cdot [\nabla \cdot (AU)] = \nabla' \cdot \nabla : (AU) \quad (12.96)$$

applied to $A(\mathbf{r}, \mathbf{r}') = N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}')$ finally results in the following tensor product sum for the diamagnetic part of the generalized response tensor:

$$\frac{ie^2}{m\omega} N_0(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \mathbf{U} = \frac{1}{i\omega} \sum_{I \neq J} \frac{P_J - P_I}{E_J - E_I} \mathbf{J}_{I \rightarrow J}^0(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}'). \quad (12.97)$$

When (12.97) is inserted in (12.79) it appears that the response tensor can be written in the compact form

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{\hbar}{i} \sum_{I \neq J} \frac{P_J - P_I}{E_J - E_I} \frac{1}{\hbar\omega + E_J - E_I} \mathbf{J}_{I \rightarrow J}^0(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}'). \quad (12.98)$$

The sum of the para- and diamagnetic contributions hence does not diverge in the low-frequency limit:

$$\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow 0) = \frac{\hbar}{i} \sum_{I \neq J} \frac{P_J - P_I}{(E_J - E_I)^2} \mathbf{J}_{I \rightarrow J}^0(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^0(\mathbf{r}'). \quad (12.99)$$

In the limit $\omega \rightarrow 0$ all transverse electric fields disappear, and $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow 0)$ thus is the response tensor associated with static longitudinal external fields, $\mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega \rightarrow 0)$. In the static limit, the equation of continuity show that all current densities must be transverse, i.e., $\mathbf{J}(\mathbf{r}; \omega \rightarrow 0) = \mathbf{J}_T(\mathbf{r}; \omega \rightarrow 0)$. In consequence, $\nabla \cdot \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow 0) = 0$. So-called persistent current densities, of interest for instance in relation to possible observations of the Aharonov–Bohm effect in angular momentum photon drag [40, 42], may exist in the limit $\omega \rightarrow 0$.

12.4 Gauge Invariance of the Linearized Response

In our derivation of the many-body expression for the generalized linear response tensor $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ (12.98), we used for the external electromagnetic field a gauge in which $\phi^{\text{ext}} = 0$. The question therefore naturally arises whether the expression

obtained for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ is independent of the gauge choice made for the prescribed field. Although quantum electrodynamics as such is a gauge invariant theory it is perhaps not obvious that the linearization of the current density response does not lead to a breaking of the gauge invariance principle. Fortunately, this principle survives the linearization process, as I shall demonstrate below. The gauge invariance of the expression we have obtained for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ is of great importance in relation to fundamental studies of local-field effects in mesoscopic optics and near-field electrodynamics. Since the transverse part of the vector potential is unaffected by a gauge transformation it is necessary only to prove the gauge invariance for a longitudinal external stimulus.

The starting point for our analysis hence is the constitutive relation

$$\mathbf{J}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega) d^3 r', \quad (12.100)$$

with

$$\mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega) = i\omega \mathbf{A}_L^{\text{ext}}(\mathbf{r}; \omega) - \nabla \phi^{\text{ext}}(\mathbf{r}; \omega), \quad (12.101)$$

and the fact that the expression for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ (12.98) was obtained in a Hamiltonian description with $\mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega) = i\omega \mathbf{A}_L^{\text{ext}}(\mathbf{r}; \omega)$, i.e., in a $\phi^{\text{ext}}(\mathbf{r}; \omega) = 0$ -gauge. With the help of the equation of continuity

$$\nabla \cdot \mathbf{J}(\mathbf{r}; \omega) + ie\omega N(\mathbf{r}; \omega) = 0, \quad (12.102)$$

where $N(\mathbf{r}; \omega)$ is the induced particle density in the frequency domain, one may easily obtain a nonlocal relation between $N(\mathbf{r}; \omega)$ and $\mathbf{E}_L^{\text{ext}}(\mathbf{r}; \omega)$ by combining (12.100) and (12.102). *Provided* we tentatively assume that the expression we have obtained for $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ (12.98) is gauge invariant, substitution of

$$\mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega) = -\nabla' \phi^{\text{ext}}(\mathbf{r}'; \omega) \quad (12.103)$$

in (12.100) thereafter allows one to obtain a nonlocal relation between $N(\mathbf{r}; \omega)$ and $\phi^{\text{ext}}(\mathbf{r}; \omega)$. Thus,

$$N(\mathbf{r}; \omega) = \frac{1}{ie\omega} \int_{-\infty}^{\infty} [\nabla \cdot \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)] \cdot \nabla' \phi^{\text{ext}}(\mathbf{r}'; \omega) d^3 r'. \quad (12.104)$$

Since $\mathbf{S}$ vanishes outside the electron system integration by parts leads to the nonlocal relation

$$N(\mathbf{r}; \omega) = \frac{i}{e\omega} \int_{-\infty}^{\infty} [\nabla' \nabla : \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)] \phi^{\text{ext}}(\mathbf{r}'; \omega) d^3 r'. \quad (12.105)$$

Starting from a gauge in which $\mathbf{A}_L^{\text{ext}}(\mathbf{r}; \omega) = \mathbf{0}$ we establish below an alternative relation between $N(\mathbf{r}; \omega)$ and $\phi^{\text{ext}}(\mathbf{r}; \omega)$, viz.,

$$N(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \chi(\mathbf{r}, \mathbf{r}'; \omega) \phi^{\text{ext}}(\mathbf{r}'; \omega) d^3 r', \quad (12.106)$$

where $\chi(\mathbf{r}, \mathbf{r}'; \omega)$ is the so-called many-body density–density response function. The reason for this name will become obvious when its explicit expression is given. The response tensor $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ often is called the many-body current–current response function because its tensor product structure involves matrix elements of two current–density operators, $\hat{\mathbf{j}}_0(\mathbf{r})$ and $\hat{\mathbf{j}}_0(\mathbf{r}')$, cf. (12.77) and (12.98). In order for the formalism to be gauge invariant, it is required that the current–current and density–density response functions satisfy the relation

$$\chi(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{e\omega} \nabla' \nabla : \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega), \quad (12.107)$$

χ being calculated in a $\mathbf{A}_{\text{L}}^{\text{ext}} = \mathbf{0}$ -gauge, and $\mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega)$ in a $\phi^{\text{ext}} = 0$ -gauge, as already emphasized. In view of the linearity of our response formalism, it is sufficient for the proof of gauge invariance to calculate the response of the system to pure scalar (ϕ^{ext}) and pure vector ($\mathbf{A}_{\text{L}}^{\text{ext}}$) potentials.

Let us consider the right-hand side of (12.107). By utilizing (12.94) one obtains after a few elementary calculations

$$\begin{aligned} & \frac{i}{e\omega} \nabla' \nabla : \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) \\ &= -\frac{e}{\hbar\omega} \sum_{I,J} \frac{(P_J - P_I)(E_I - E_J)}{\hbar\omega + E_J - E_I} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle. \end{aligned} \quad (12.108)$$

For what follows it is useful to rewrite this equation in the form

$$\begin{aligned} & \frac{i}{e\omega} \nabla' \nabla : \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) \\ &= -e \sum_{I,J} \frac{(P_J - P_I)}{\hbar\omega + E_J - E_I} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle \\ & \quad + e \sum_{I,J} \frac{P_J - P_I}{\hbar\omega} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle. \end{aligned} \quad (12.109)$$

The last double sum in (12.109) is zero, as the reader may realize by rewriting it as follows:

$$\begin{aligned} & \sum_{I,J} (P_J - P_I) \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle = \sum_J P_J \langle J | \hat{n}(\mathbf{r}) [\sum_I | I \rangle \langle I |] \hat{n}(\mathbf{r}') | J \rangle \\ & \quad - \sum_I P_I \langle I | \hat{n}(\mathbf{r}') [\sum_J | J \rangle \langle J |] \hat{n}(\mathbf{r}) | I \rangle = \sum_J P_J \langle J | [\hat{n}(\mathbf{r}), \hat{n}(\mathbf{r}')] | J \rangle. \end{aligned} \quad (12.110)$$

The last equality in (12.110) follows by use of the completeness relation, and there-upon a dummy variable interchange $I \rightleftharpoons J$ in the sum containing P_I . Since the particle number operators commute, i.e.,

$$[\hat{n}(\mathbf{r}), \hat{n}(\mathbf{r}')] = 0 \quad (12.111)$$

the last double sum in (12.109) vanishes, q.e.d. For the right side of (12.107) we have hence gotten the expression

$$\frac{i}{e\omega} \nabla' \nabla : \mathbf{S}(\mathbf{r}, \mathbf{r}'; \omega) = -e \sum_{I,J} \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle. \quad (12.112)$$

Let us next calculate the density–density response function. The relation between $N(\mathbf{r}; \omega)$ and $\phi^{\text{ext}}(\mathbf{r}'; \omega)$ in (12.106) is obtained from

$$N(\mathbf{r}; \rho) = \text{Tr} \{ \hat{\rho}_1(\omega) \hat{n}(\mathbf{r}) \} = \sum_{I,J} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{\rho}_1(\omega) | J \rangle, \quad (12.113)$$

which, with use of (12.46), can be written in the form

$$N(\mathbf{r}; \omega) = \sum_{I,J} \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{H}_1(\omega) | J \rangle. \quad (12.114)$$

In the gauge in which $\mathbf{A}^{\text{ext}} = \mathbf{0}$ one has

$$\hat{H}_1(\omega) = -e \sum_{\alpha} \phi^{\text{ext}}(\mathbf{r}_{\alpha}; \omega) = -e \int_{-\infty}^{\infty} \hat{n}(\mathbf{r}') \phi^{\text{ext}}(\mathbf{r}'; \omega) d^3 r', \quad (12.115)$$

since the number operator is given by (12.82). The IJ th matrix element of $\hat{H}_1(\omega)$, therefore is given by

$$\langle I | \hat{H}_1(\omega) | J \rangle = -e \int_{-\infty}^{\infty} \langle I | \hat{n}(\mathbf{r}') | J \rangle \phi^{\text{ext}}(\mathbf{r}'; \omega) d^3 r'. \quad (12.116)$$

By combining (12.114) and (12.116), one immediately obtain upon a comparison to (12.106) the following formula for the density–density response function

$$\chi(\mathbf{r}, \mathbf{r}'; \omega) = -e \sum_{I,J} \frac{P_J - P_I}{\hbar\omega + E_J - E_I} \langle J | \hat{n}(\mathbf{r}) | I \rangle \langle I | \hat{n}(\mathbf{r}') | J \rangle. \quad (12.117)$$

Since the right-hand sides of (12.112) and (12.117) are identical, the gauge invariance condition in (12.107) is indeed satisfied. The term density–density response function now is seen to make sense because the expression given for $\chi(\mathbf{r}, \mathbf{r}'; \omega)$ in (12.117) contains two particle density operators $\hat{n}(\mathbf{r})$ and $\hat{n}(\mathbf{r}')$ in the various terms.

12.5 Remarks on the Low- and High-Frequency Responses

In relation to the discussion of the general linear constitutive relation in Sect. 10.7, four so-called dyadic delta function projections of the generalized response tensor were introduced, see (10.80). In the case where the particle system exhibits translational invariance in time explicit expressions for the various response tensors $\mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}'; \omega)$ (A and B equal to T or L) can be set up. If the transverse and longitudinal parts of the many-body transition current density $\mathbf{J}_{I \rightarrow J}^0$ ($\mathbf{J}_{J \rightarrow I}^0$) are denoted by $\mathbf{J}_{I \rightarrow J}^T$ ($\mathbf{J}_{J \rightarrow I}^T$) and $\mathbf{J}_{I \rightarrow J}^L$ ($\mathbf{J}_{J \rightarrow I}^L$), one immediately obtains from (12.98) the result

$$\mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{\hbar}{i} \sum_{I \neq J} \frac{P_J - P_I}{E_J - E_I} \frac{1}{\hbar\omega + E_J - E_I} \mathbf{J}_{I \rightarrow J}^A(\mathbf{r}) \mathbf{J}_{J \rightarrow I}^B(\mathbf{r}'). \quad (12.118)$$

By means of the projections, $\mathbf{S}_{AB}$, the constitutive relations for the T and L parts of the induced current density can be written as follows:

$$\mathbf{J}_T(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} (\mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T(\mathbf{r}'; \omega) + \mathbf{S}_{TL}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega)) d^3 r', \quad (12.119)$$

$$\mathbf{J}_L(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} (\mathbf{S}_{LT}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T(\mathbf{r}'; \omega) + \mathbf{S}_{LL}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega)) d^3 r', \quad (12.120)$$

Since $\nabla \times \mathbf{E}_T(\mathbf{r}; \omega \rightarrow 0) = \mathbf{0}$, cf. (9.25), and $\nabla \cdot \mathbf{E}_T(\mathbf{r}; \omega) = 0$ per definition, the transverse part of the electric field vanishes in the low frequency limit. The transverse part of the current density does not vanish in this limit, neither does the magnetic field. For $\omega \rightarrow 0$, the constitutive relation in (12.119) hence takes the form

$$\mathbf{J}_T(\mathbf{r}; \omega \rightarrow 0) = \int_{-\infty}^{\infty} (\mathbf{S}_{TL}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow 0) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}'; \omega \rightarrow 0)) d^3 r'. \quad (12.121)$$

The current density in (12.121) gives rise to an induced static magnetic field

$$\mathbf{B}(\mathbf{r}; \omega \rightarrow 0) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-1} \nabla' \times \mathbf{J}_T(\mathbf{r}'; \omega \rightarrow 0) d^3 r'. \quad (12.122)$$

This well-known result follows directly from the forced part of the solution to the Helmholtz equation for the magnetic field (3.50) in the magnetostatic limit.

It appears from a comparison of (12.97) and (12.98) that at sufficiently high frequencies, i.e., frequencies for which $\hbar\omega \gg |E_J - E_I|$ for all I and J , the response tensor becomes identical with its diamagnetic part. The diamagnetic part of $\mathbf{S}$ is proportional to ω^{-1} for all frequencies. If the diamagnetic response tensor, given in its spatially local form (see (12.79)), is inserted into (10.80) one obtains

$$\mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow \infty) = \frac{ie^2}{m\omega} \int_{-\infty}^{\infty} N_0(\mathbf{r}'') \delta_A(\mathbf{r} - \mathbf{r}'') \cdot \delta_B(\mathbf{r}'' - \mathbf{r}') d^3 r''. \quad (12.123)$$

For an inhomogeneous electron distribution all four combinations of $\mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow \infty)$ will be nonvanishing in general. If the distribution is homogeneous one gets

$$\begin{aligned} \mathbf{S}_{AB}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow \infty) &= \frac{ie^2 N_0}{m\omega} \int_{-\infty}^{\infty} \boldsymbol{\delta}_A(\mathbf{r} - \mathbf{r}'') \cdot \boldsymbol{\delta}_B(\mathbf{r}'' - \mathbf{r}') d^3 r'' \\ &= \frac{ie^2 N_0}{m\omega} \boldsymbol{\delta}_A(\mathbf{r} - \mathbf{r}') \delta_{AB}. \end{aligned} \quad (12.124)$$

Hence, only the response tensors $\mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow \infty)$ and $\mathbf{S}_{LL}(\mathbf{r}, \mathbf{r}'; \omega \rightarrow \infty)$ are different from zero in this particular case, as expected.

Chapter 13

Microscopic Ewald–Oseen Extinction Theorem: Coupled-Antenna Theory

13.1 Extinction Theorem for Transverse Dynamics

13.1.1 Integral Relation Between Field and Current Density

We know from (9.30) that the transverse part of the electric field satisfies the inhomogeneous vectorial Helmholtz equation

$$(\nabla^2 + q_0^2)\mathbf{E}_T(\mathbf{r}; \omega) = -i\mu_0\omega\mathbf{J}_T(\mathbf{r}; \omega) \quad (13.1)$$

in the space–frequency domain. In the quantum domain, $\mathbf{J}_T(\mathbf{r}; \omega)$ is the timely Fourier transform of the quantum mechanical mean value of the transverse part of the current density operator in the given pure or mixed state. As such, $\mathbf{J}_T(\mathbf{r}; \omega)$ may be considered as a continuum field without singularities. In the classical domain, where the particles are point entities, the transverse part of the current density is singular at the positions of the various charges. Outside the singular point given by $|\mathbf{r} - \mathbf{r}'| = 0$, the scalar propagator satisfies the homogeneous Helmholtz equation

$$(\nabla^2 + q_0^2)g(|\mathbf{r} - \mathbf{r}'|; \omega) = 0 \quad (13.2)$$

in the $(\mathbf{r}, \omega)$ -domain, see (3.42). The transverse current density $\mathbf{J}_T(\mathbf{r}; \omega)$ is nonvanishing not only inside matter (the region where $\mathbf{J}(\mathbf{r}; \omega) \neq \mathbf{0}$ we denote by V) but also in the rim zone of matter where $\mathbf{J}_T(\mathbf{r}; \omega) = -\mathbf{J}_L(\mathbf{r}; \omega) \neq \mathbf{0}$, see Sect. 9.2.2. The spatial domain in which the transverse current density is different from zero is in the following denoted V_T . There is of course no sharp boundary for V_T in the quantum case, and it is therefore better to characterize V_T as the volume outside which $\mathbf{J}_T(\mathbf{r}; \omega)$ *effectively* can be neglected in a given calculation. Although the relative difference $(V_T - V)/V$ is small for macroscopic media, it is usually quite large for mesoscopic and microscopic objects. For electrically neutral objects so small that a multiple expansion of $\mathbf{J}_T(\mathbf{r}; \omega)$ is useful, the transverse current density associated with electric dipole radiation decays asymptotically as R^3 , where R is the distance from the dipole. In this case, one must be careful with the choice of the

effective V_T . Independent of it is relative size the rim zone is always of importance in near-field electrodynamics, ipso-facto that the near field zone is the rim zone. The closed surface bounding V_T is in the following denoted Σ_T .

By means of Green's theorem, applied to the functions $\mathbf{E}_T(\mathbf{r}; \omega)$ and $g(|\mathbf{r} - \mathbf{r}'|; \omega)$, we shall now establish a fruitful integral relation between the transverse parts of the electric field and current density distribution. To lighten the notation the reference to ω is omitted in most of the following equations in Sect. 13.1. As a starting point we take the following identity

$$\begin{aligned} \nabla' \cdot [E_{T,i}(\mathbf{r}') \nabla' g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) \nabla' E_{T,i}(\mathbf{r}')] \\ = E_{T,i}(\mathbf{r}') (\nabla')^2 g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) (\nabla')^2 E_{T,i}(\mathbf{r}'), \quad i = x, y, z, \end{aligned} \quad (13.3)$$

where $E_{T,i}$ is the i th Cartesian component of $\mathbf{E}_T(\mathbf{r}')$. Since the Huygens propagator is singular at $\mathbf{r} = \mathbf{r}'$, one must omit this point from the domain of integration which enters Green's theorem. Thus, we cut out from the domain a small spherical exclusion volume $\epsilon(\mathbf{r})$ centered on the point $\mathbf{r}$ inside V_T at which we want to calculate $\mathbf{E}_T(\mathbf{r})$. The surface and radius of the sphere are denoted by σ and s , respectively. The domain of integration, and the notation used, are shown in Fig. 13.1. Near the end of our calculation we take the limit $s \rightarrow 0$. Although the form of the exclusion volume cannot have any physical importance, we have chosen a spherical exclusion volume for two reasons: (1) Certain technical calculations become easy to carry out and (2) a “simple physical picture” based on propagators which describe isotropic field propagation in space emerges (see Sect. 13.3). Upon integration of (13.3) over the volume between the surface Σ_T and σ , and use of Gauss' theorem to the integral on the left-hand side of the resulting equation, one obtains

$$\begin{aligned} \int_{\Sigma_T + \sigma} \hat{\mathbf{n}}(\mathbf{r}') \cdot [E_{T,i}(\mathbf{r}') \nabla' g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) \nabla' E_{T,i}(\mathbf{r}')] dS' \\ = \int_{\epsilon(\mathbf{r})}^{V_T} [E_{T,i}(\mathbf{r}') (\nabla')^2 g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) (\nabla')^2 E_{T,i}(\mathbf{r}')] d^3 r', \end{aligned} \quad (13.4)$$

where $\hat{\mathbf{n}}(\mathbf{r}')$ is a unit normal vector at the point $\mathbf{r}'$ (located on Σ_T or σ). At every point $\hat{\mathbf{n}}(\mathbf{r}')$ is directed away from the integration volume. By utilizing the i th component of (13.1) and (13.2) we have

$$\begin{aligned} \int_{\epsilon(\mathbf{r})}^{V_T} [E_{T,i}(\mathbf{r}') (\nabla')^2 g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) (\nabla')^2 E_{T,i}(\mathbf{r}')] d^3 r' \\ = i\mu_0\omega \int_{\epsilon(\mathbf{r})}^{V_T} g(|\mathbf{r} - \mathbf{r}'|) J_{T,i}(\mathbf{r}') d^3 r'. \end{aligned} \quad (13.5)$$

By multiplication of this equation by the unit vector in the i -direction, and thereafter addition of the equations for $i = x, y$, and z , one gets after slight rearrangements

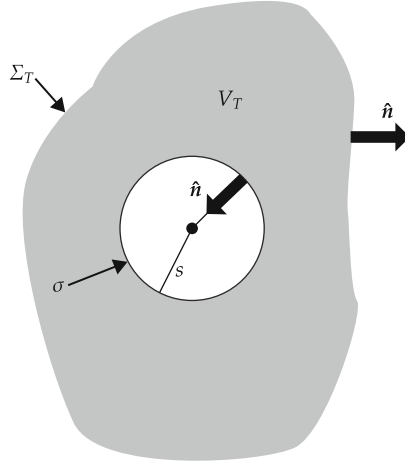


Fig. 13.1 Schematic illustration showing important quantities used in the application of Green's theorem to the functions $E_T(\mathbf{r}; \omega)$ and $g(|\mathbf{r} - \mathbf{r}'|; \omega)$. The integration is over the (rim zone) domain V_T where the transverse current density *effectively* is nonvanishing. The closed boundary of V_T is denoted by Σ_T . Since the Huygens scalar propagator, $g(|\mathbf{r} - \mathbf{r}'|; \omega)$, is singular at $\mathbf{r}' = \mathbf{r}$, a small spherical volume of radius s , and centered on $\mathbf{r}$, is cut out from the domain of integration. The spherical surface is denoted by σ . The “outwards” directed unit vector on Σ_T and σ is called $\hat{n}$. At the end of the calculation the limit $s \rightarrow 0$ is taken

$$\begin{aligned} & \int_{\Sigma_T + \sigma} [E_T(\mathbf{r}') \hat{n}(\mathbf{r}') \cdot \nabla' g(|\mathbf{r} - \mathbf{r}'|) - g(|\mathbf{r} - \mathbf{r}'|) (\hat{n}(\mathbf{r}') \cdot \nabla') E_T(\mathbf{r}')] dS' \\ &= i\mu_0\omega \int_{\epsilon(\mathbf{r})}^{V_T} g(|\mathbf{r} - \mathbf{r}'|) J_{T,i}(\mathbf{r}') d^3r'. \end{aligned} \quad (13.6)$$

An explicit calculation of the integral over the surface σ can be carried out in the limit $s \rightarrow 0$. We start from the equations

$$\begin{aligned} & \lim_{s \rightarrow 0} \left\{ \int_{\sigma} E_T(\mathbf{r}') \hat{n}(\mathbf{r}') \cdot \nabla' g(|\mathbf{r} - \mathbf{r}'|) dS' \right\} \\ &= E_T(\mathbf{r}) \lim_{s \rightarrow 0} \left\{ \int_{\sigma} \hat{n}(\mathbf{r}') \cdot \nabla' g(|\mathbf{r} - \mathbf{r}'|) dS' \right\}, \end{aligned} \quad (13.7)$$

$$\begin{aligned} & \lim_{s \rightarrow 0} \left\{ \int_{\sigma} g(|\mathbf{r} - \mathbf{r}'|) (\hat{n}(\mathbf{r}') \cdot \nabla') E_T(\mathbf{r}') dS' \right\} \\ &= \left[\lim_{s \rightarrow 0} \left\{ \int_{\sigma} g(|\mathbf{r} - \mathbf{r}'|) \hat{n}(\mathbf{r}') dS' \right\} \right] \cdot \nabla E_T(\mathbf{r}), \end{aligned} \quad (13.8)$$

and with the help of the relation $[R = |\mathbf{r} - \mathbf{r}'|]$

$$\nabla' g(|\mathbf{r} - \mathbf{r}'|) = -\hat{n}(\mathbf{r}') \frac{\partial g(R)}{\partial R}, \quad (13.9)$$

we obtain

$$\begin{aligned} \lim_{s \rightarrow 0} \left\{ \int^{\sigma} \hat{\mathbf{n}}(\mathbf{r}') \cdot \nabla' g(|\mathbf{r} - \mathbf{r}'|) dS' \right\} &= - \lim_{s \rightarrow 0} \left\{ \int^{\sigma} \frac{\partial g(R)}{\partial R} dS' \right\} \\ &= - \lim_{s \rightarrow 0} \left\{ \frac{1}{4\pi} \left(\frac{iq_0}{s} - \frac{1}{s^2} \right) e^{iq_0 s} 4\pi s^2 \right\} = 1. \end{aligned} \quad (13.10)$$

The first part (13.7) of the integral over σ thus gives $\mathbf{E}_T(\mathbf{r})$ in the limit $s \rightarrow 0$. Since,

$$\int^{\sigma} g(R) \hat{\mathbf{n}}(\mathbf{r}') dS' = g(R) \int^{\sigma} \hat{\mathbf{n}}(\mathbf{r}') dS' = \mathbf{0}, \quad (13.11)$$

the second part (13.8) vanishes in the limit. The explicit result $\mathbf{E}_T(\mathbf{r})$ for the integral over σ implies that (13.6) for $s \rightarrow 0$ takes the form

$$\mathbf{E}_T(\mathbf{r}) = \boldsymbol{\Sigma}_T(\mathbf{r}) + i\mu_0\omega \int_{\epsilon(\mathbf{r}) \rightarrow 0}^{V_T} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T(\mathbf{r}') d^3r', \quad \mathbf{r} \in V_T, \quad (13.12)$$

where

$$\boldsymbol{\Sigma}_T(\mathbf{r}) = \int^{\Sigma_T} [g(|\mathbf{r} - \mathbf{r}'|) \hat{\mathbf{n}} \cdot \nabla' \mathbf{E}_T(\mathbf{r}') - \mathbf{E}_T(\mathbf{r}') \hat{\mathbf{n}} \cdot \nabla' g(|\mathbf{r} - \mathbf{r}'|)] dS'. \quad (13.13)$$

As indicated, the integral relation between the transverse parts of the electric field and the current density given in (13.12) holds for observation point $\mathbf{r}$ located inside V_T .

13.1.2 Ewald–Oseen Extinction Theorem

The dynamics of the particles in V_T is driven by the electrodynamic field generated by a system of external (source) charges. Let us assume that the transverse part $\mathbf{J}_T^{\text{ext}}(\mathbf{r}; \omega) \equiv \mathbf{J}_T^{\text{ext}}(\mathbf{r})$ of these charges occupies a volume V_T^{ext} , and is bounded by a closed surface denoted by Σ_T^{ext} . In the following we demand that the domains V_T and V_T^{ext} do not overlap in space (Fig. 13.2). The source-system coupling hence is not a near-field coupling, and only the radiative part of the electromagnetic field brings about the coupling. The vacuum domain outside V_T^{ext} and V_T is denoted by $\tilde{V}_T$.

If the point of observation lies outside V_T , i.e., in $\tilde{V}_T$ or V_T^{ext} , Green's theorem applied once again to V_T gives

$$\mathbf{0} = \boldsymbol{\Sigma}_T(\mathbf{r}) + i\mu_0\omega \int^{V_T} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T(\mathbf{r}') d^3r', \quad \mathbf{r} \in \tilde{V}_T \text{ or } V_T^{\text{ext}}, \quad (13.14)$$

since $g(|\mathbf{r} - \mathbf{r}'|)$ has no singularity in this case, and the surface integral over σ therefore is absent. If Green's theorem is applied to the vacuum domain $\tilde{V}_T$, where

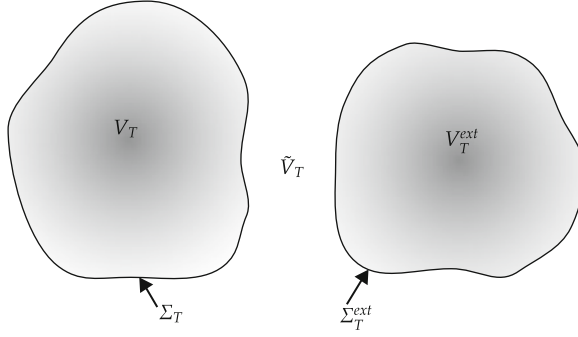


Fig. 13.2 Schematic illustration of the transverse current density domains of the external source charges (V_T^{ext}) and the charge system under study (V_T). The surfaces enclosing these domains are denoted by Σ_T^{ext} and Σ_T , and for the space outside the notation $\tilde{V}_T$ is employed. Green's theorem applied in turn to the three domains V_T , $\tilde{V}_T$, and V_T^{ext} results in six important relations, and from these a microscopic Ewald–Oseen extinction theorem is obtained

$\mathbf{J}_T$ and $\mathbf{J}_T^{\text{ext}}$ are both zero, two equations analogous to (13.12) and (13.14) are obtained, viz.

$$\mathbf{E}_T(\mathbf{r}) = -\boldsymbol{\Sigma}_T(\mathbf{r}) - \boldsymbol{\Sigma}_T^{\text{ext}}(\mathbf{r}), \quad \mathbf{r} \in \tilde{V}_T, \quad (13.15)$$

$$\mathbf{0} = -\boldsymbol{\Sigma}_T(\mathbf{r}) - \boldsymbol{\Sigma}_T^{\text{ext}}(\mathbf{r}), \quad \mathbf{r} \in V_T \text{ or } V_T^{\text{ext}}. \quad (13.16)$$

In these equations, $\boldsymbol{\Sigma}_T^{\text{ext}}$ has the form given in (13.13) with the integration extending over the surface Σ_T^{ext} . The minus signs in front of $\boldsymbol{\Sigma}_T(\mathbf{r})$ and $\boldsymbol{\Sigma}_T^{\text{ext}}$ in (13.15) and (13.16) arise from the fact that the unit normal vectors $\hat{\mathbf{n}}$ on the Σ_T - and Σ_T^{ext} -surface point *into* the vacuum domain. Let us finally apply Green's theorem to the source domain V_T^{ext} . In this domain, the current density $\mathbf{J}_T^{\text{ext}}$ is nonvanishing, and from the analogy to (13.12) and (13.14) it follows immediately that

$$\mathbf{E}_T(\mathbf{r}) = \boldsymbol{\Sigma}_T^{\text{ext}}(\mathbf{r}) + i\mu_0\omega \int_{\epsilon(\mathbf{r}) \rightarrow 0}^{V_T^{\text{ext}}} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T^{\text{ext}}(\mathbf{r}') d^3r', \quad \mathbf{r} \in V_T^{\text{ext}}, \quad (13.17)$$

$$\mathbf{0} = \boldsymbol{\Sigma}_T^{\text{ext}}(\mathbf{r}) + i\mu_0\omega \int_{V_T^{\text{ext}}} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T^{\text{ext}}(\mathbf{r}') d^3r', \quad \mathbf{r} \in V_T \text{ or } \tilde{V}_T. \quad (13.18)$$

The use of Green's theorem to the domains V_T , $\tilde{V}_T$, and V_T^{ext} thus has led to the six important equations in (13.12), and (13.14)–(13.18).

How can one interpret the quantity $\boldsymbol{\Sigma}_T(\mathbf{r})$ in (13.13) from a physical point of view? To answer this question we add (13.16) and (13.18), and note that the addition is only possible if $\mathbf{r} \in V_T$. Hence we obtain

$$\Sigma_T(\mathbf{r}) = i\mu_0\omega \int_{V_T^{\text{ext}}} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T^{\text{ext}}(\mathbf{r}') d^3r', \quad \mathbf{r} \in V_T. \quad (13.19)$$

Since the right side of (13.19) may be identified as the transverse electric field from the source, i.e.,

$$\mathbf{E}_T^{\text{ext}}(\mathbf{r}) = i\mu_0\omega \int_{V_T^{\text{ext}}} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T^{\text{ext}}(\mathbf{r}') d^3r', \quad \mathbf{r} \in \tilde{V}_T \text{ or } V_T \quad (13.20)$$

it appears that

$$\Sigma_T(\mathbf{r}) = \mathbf{E}_T^{\text{ext}}, \quad \mathbf{r} \in V_T. \quad (13.21)$$

The term $\Sigma_T(\mathbf{r})$ in (13.12) thus equals the transverse external electric field acting on our system. The result in (13.21) is an example of a microscopic Ewald–Oseen extinction theorem. Extinctions theorems equivalently to the one above can be established for the domains V_T^{ext} and $\tilde{V}_T$. In the classical formulation of the Ewald–Oseen extinction theorem [43, 282, 283] in molecular optics it is asserted that the incident field is extinguished by those molecular dipoles that are situated on the boundary of the dielectric medium in consideration. A generalization of the classical extinction theory, originally derived from molecular optics, which is kind of classical microscopic theory, has been provided by Wolf and others [284–287]. In the generalized approach of Wolf, the extinction theorem is derived from the macroscopic Maxwell equations and the theorem is shown to hold for media with a quite arbitrary macroscopic response. In the form given above the microscopic Ewald–Oseen theorem holds even in the quantum regime, and it has been used also in nonlinear surface optics [288]. It is possible to establish microscopic extinction theorems also in the case where the domains V_T and V_T^{ext} overlap in space. Such a generalization will not be discussed here, nor is it needed in what follows.

13.2 Integral Equations

By combining (13.12) and (13.21) one obtains

$$\mathbf{E}_T(\mathbf{r}) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}) + i\mu_0\omega \int_{V_T} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T(\mathbf{r}') d^3r', \quad \mathbf{r} \in V_T, \quad (13.22)$$

in a notation where the reference “ $\epsilon(\mathbf{r}) \rightarrow 0$ ” has been omitted from the integral sign. Since $\mathbf{J}_T(\mathbf{r}')$ is nonsingular everywhere in space for physical reasons, the integral with the “weak” $|\mathbf{r} - \mathbf{r}'|^{-1}$ singularity is absolutely convergent and therefore there is no need to keep the reference at the foot of the integral sign. It appears from (13.18) and (13.20) that

$$\Sigma_T^{\text{ext}}(\mathbf{r}) = -\mathbf{E}_T^{\text{ext}}(\mathbf{r}), \quad \mathbf{r} \in V_T \text{ or } \tilde{V}_T, \quad (13.23)$$

for point outside the source domain. If the information in (13.14), (13.15), and (13.23) are combined one realizes that

$$\mathbf{E}_T(\mathbf{r}) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}) + i\mu_0\omega \int^{V_T} g(|\mathbf{r} - \mathbf{r}'|) \mathbf{J}_T(\mathbf{r}') d^3r', \quad \mathbf{r} \in \tilde{V}_T, \quad (13.24)$$

for $\mathbf{r}$ -points in the vacuum. Together, (13.22) and (13.24) show that an integral relation between $\mathbf{E}_T(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r})$ of the type

$$\mathbf{E}_T(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + i\mu_0\omega \int^{V_T} g(|\mathbf{r} - \mathbf{r}'|; \omega) \mathbf{J}_T(\mathbf{r}'; \omega) d^3r' \quad (13.25)$$

holds everywhere in space outside the source domain V_T^{ext} . This equation is just the timely Fourier transform of (10.4) since $\mathbf{J}_T(\mathbf{r}; \omega)$ is nonvanishing only in the V_T domain. By utilizing the microscopic Ewald–Oseen extinction theorem one is led back to the integral relation in (10.4), a relation most often established in a somewhat less rigorous fashion by standard Green function technique [19].

13.3 Coupled-Antenna Theory

13.3.1 Matrix Equation Problem for the Local Field

The integral equation in (13.25) relates two yet unknown vector-field distributions, viz., $\mathbf{E}_T(\mathbf{r}; \omega)$ and $\mathbf{J}_T(\mathbf{r}; \omega)$. In order to determine these distributions (13.25) must be supplemented by some sort of constitutive relation, as we know. Within the framework of linear response theory the most general relation between $\mathbf{J}_T(\mathbf{r}; \omega)$ and $\mathbf{E}_T(\mathbf{r}; \omega)$ takes the form given in (12.119). If the external sources are located outside V_T the constitutive relation is reduced to

$$\mathbf{J}_T(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega) \cdot \mathbf{E}_T(\mathbf{r}'; \omega) d^3r', \quad (13.26)$$

where

$$\mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{\hbar}{i} \sum_{K \neq L} \frac{P_L - P_K}{E_L - E_K} \frac{1}{\hbar\omega + E_L - E_K} \mathbf{J}_{K \rightarrow L}^T(\mathbf{r}) \mathbf{J}_{L \rightarrow K}^T(\mathbf{r}') \quad (13.27)$$

is the relevant many-body response tensor; see (12.118). The tensor product structure of $\mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega)$ allows to a certain extent a simplification of the constitutive relation. With the abbreviations

$$A_{KL}(\omega) = \mu_0 \frac{P_L - P_K}{E_L - E_K} \frac{\hbar\omega}{\hbar\omega + E_L - E_K}, \quad (13.28)$$

and

$$\beta_{L \rightarrow K}(\omega) = \int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^T(\mathbf{r}) \cdot \mathbf{E}_T(\mathbf{r}; \omega) d^3r, \quad (13.29)$$

one has

$$i\mu_0\omega \mathbf{J}_T(\mathbf{r}, \omega) = \sum_{K,L} A_{KL}(\omega) \mathbf{J}_{K \rightarrow L}^T(\mathbf{r}) \beta_{L \rightarrow K}(\omega), \quad (13.30)$$

with the implicit understanding that terms with $K = L$ are omitted from the double summation. Before we proceed the analysis it is worthwhile to take a look at the structure of (13.30). It appears that the transverse current density $\mathbf{J}_T(\mathbf{r}; \omega)$ [times $i\mu_0\omega$] has a spatial form determined by a weighted distribution of the transverse parts, $\mathbf{J}_{K \rightarrow L}^T$, of the various transition current densities, $\mathbf{J}_{K \rightarrow L}^0(\mathbf{r})$. The spatial forms of these parts are independent of the dynamical state of the system, and can in principle be calculated from a knowledge of the many-body wave function in the relevant (K, L) stationary states. The weight factor for the $K \rightarrow L$ transition is the product $A_{KL}(\omega)\beta_{L \rightarrow K}(\omega)$. The frequency dependent quantity $A_{KL}(\omega)$ becomes particularly large for frequencies in the vicinity of the electronic resonance frequency $(E_K - E_L)/\hbar$, [$E_K > E_L$]. With our omission of irreversible damping mechanisms $A_{KL}(\omega)$ diverges at resonance. The $A_{KL}(\omega)$ factor is in principle known once the angular frequency is given. The other factor $\beta_{L \rightarrow K}(\omega)$ in the weight product, given by the integral in (13.29), is at this stage unknown because it depends on the yet unknown local electric field, $\mathbf{E}_T(\mathbf{r}; \omega)$. The physics hidden in the $\beta_{L \rightarrow K}(\omega)$ factor may be described as follows: During a transition from state L to state K a time dependent current will in the quantum statistical sense flow in the many-electron system. The current density in the flow will be proportional to the many-body transition current density $\mathbf{J}_{L \rightarrow K}^0(\mathbf{r})$, and the factor of proportionality will be time dependent. In the local interaction with the transverse part of the electric field, the transverse part of the transition current density, $\mathbf{J}_{L \rightarrow K}^T(\mathbf{r})$, enters. At a given frequency the rate of work done locally (at $\mathbf{r}$) by the transverse part of the local electric field will be proportional to $\mathbf{J}_{L \rightarrow K}^T(\mathbf{r}) \cdot \mathbf{E}_T(\mathbf{r}; \omega)$. The $\beta_{L \rightarrow K}(\omega)$ factor is the integral of this quantity over the spatial domain occupied by the transverse transition current density, cf. the definition in (13.29). From a qualitative point of view this domain equals the V_T domain, cf. (13.30).

It is possible to shrink the integration domain for $\beta_{L \rightarrow K}(\omega)$, to the in general much smaller domain occupied by $\mathbf{J}_{L \rightarrow K}^0(\mathbf{r})$. In order to realize this, one may make use of the orthogonality relation

$$\mathbf{W}_L(\mathbf{q}) \cdot \mathbf{W}_T(-\mathbf{q}) = 0, \quad (13.31)$$

a relation which follows immediately from the algebraic equations in (9.11) and (9.12). Hence, one obtains

$$\int_{-\infty}^{\infty} \mathbf{J}_L \rightarrow K^L(\mathbf{r}) \cdot \mathbf{E}_T(\mathbf{r}; \omega) d^3r = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^L(\mathbf{q}) \cdot \mathbf{E}_T(-\mathbf{q}, \omega) d^3q = 0, \quad (13.32)$$

where $\mathbf{J}_{L \rightarrow K}^L$ is the longitudinal part of $\mathbf{J}_{L \rightarrow K}^0$. By addition of (13.29) and (13.32), one now gets

$$\beta_{L \rightarrow K}(\omega) = \int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^0(\mathbf{r}) \cdot \mathbf{E}_T(\mathbf{r}; \omega) d^3r, \quad (13.33)$$

with an integration over the $\mathbf{J}_{L \rightarrow K}^0$ domain, q.e.d.

After this brief analysis of the constitutive equation we turn our attention towards the integral equation for the local field. By inserting (13.30) in (13.25) one obtains

$$\mathbf{E}_T(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + \sum_{K,L} \mathbf{F}_{K \rightarrow L}^T(\mathbf{r}; \omega) \beta_{L \rightarrow K}(\omega), \quad (13.34)$$

where

$$\mathbf{F}_{K \rightarrow L}^T(\mathbf{r}; \omega) = A_{KL}(\omega) \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \mathbf{J}_{K \rightarrow L}^T(\mathbf{r}') d^3r'. \quad (13.35)$$

The physical interpretation of the result in (13.34) is simple and interesting. Hence, to obtain the transverse part of the local electric field at $\mathbf{r}$, one must add to the transverse external field the transverse part of the induced field. The induced field consists of individual contribution from the various electronic (many-body) transitions. For a given pair of states, say K and L , one has two field contributions: one related to the $K \rightarrow L$ transition, and one to the opposite transition $L \rightarrow K$. The strengths of the two contributions will in general not be the same. Thus, if it is assumed that $E_L < E_K$, it appears from the expression for $A_{KL}(\omega)$ (13.28) that the transition $K \rightarrow L$ gives a much larger contribution than the $L \rightarrow K$ transition for frequencies near the electronic resonance frequency. A schematic illustration related to the considerations above is shown in Fig. 13.3. The reader should be aware of the fact that our analysis is based on *linear* response theory. Near resonance the system may react in a nonlinear fashion and, if so, the local-field calculation presented above must be abandoned. Let us now consider the $K \rightarrow L$ transition in more detail. During this

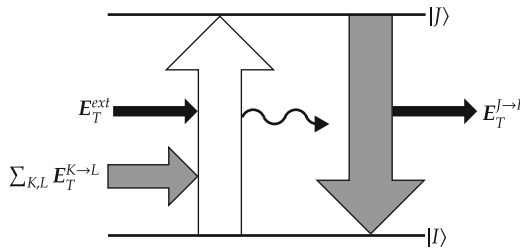


Fig. 13.3 A many-body quantum system is excited from the stationary state $|I\rangle$ to the state $|J\rangle$ by the transverse external field (E_T^{ext}) plus the sum of the transverse parts of the fields generated in all other ($K \rightarrow L$) transitions ($E_T^{K \rightarrow L}$). In the deexcitation from $|J\rangle$ to $|I\rangle$, a transverse field $E_T^{J \rightarrow I}$ is emitted in an overall energy-conserving resonant process. The (virtual) anti-resonant field emission accompanying the upwards $|I\rangle \rightarrow |J\rangle$ transition is indicated by the wavy line

transition a transverse current density with the spatial form $\mathbf{J}_{K \rightarrow L}^T(\mathbf{r}')$ is flowing. Each infinitesimal volume element d^3r' located at $\mathbf{r}'$, gives a contribution to the transverse electric field at the observation point $\mathbf{r}$. The field radiation from $\mathbf{r}'$ to $\mathbf{r}$ propagates in space in a manner described in the frequency domain by the Huygens propagator $g(|\mathbf{r} - \mathbf{r}'|; \omega)$, cf. (13.35). The total contribution to the field at $\mathbf{r}$ from the $K \rightarrow L$ transition is obtained by integration over the entire $\mathbf{J}_{K \rightarrow L}^T(\mathbf{r}')$ domain. The amplitude of this contribution cannot be given at this stage of the calculation because it depends on the yet unknown $\beta_{L \rightarrow K}(\omega)$ factor, see (13.34). To determine $\beta_{L \rightarrow K}(\omega)$ one needs to know the local field $\mathbf{E}_T$ acting on the current density distribution $\mathbf{J}_{L \rightarrow K}^T(\mathbf{r})$, cf. (13.29). This field in turn is the sum of the external field and the fields from all other transitions. The different transitions hence are coupled together by the induced local field, like a system of antennas. To determine the various $\beta_{J \rightarrow I}(\omega)$'s in a selfconsistent manner we start from (13.29), replacing $L \rightarrow K$ by $J \rightarrow I$. By inserting the expression given in (13.34) for $\mathbf{E}_T(\mathbf{r}; \omega)$ into (13.29) we obtain

$$\beta_{J \rightarrow I}(\omega) - \sum_{K,L} N_{K \rightarrow L}^{J \rightarrow I}(\omega) \beta_{L \rightarrow K}(\omega) = H_{J \rightarrow I}(\omega), \quad (13.36)$$

where

$$N_{K \rightarrow L}^{J \rightarrow I}(\omega) = A_{KL}(\omega) \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \mathbf{J}_{J \rightarrow I}^T(\mathbf{r}) \cdot \mathbf{J}_{K \rightarrow L}^T(\mathbf{r}') d^3r' d^3r, \quad (13.37)$$

and

$$H_{J \rightarrow I}(\omega) = \int_{-\infty}^{\infty} \mathbf{J}_{J \rightarrow I}^T(\mathbf{r}) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) d^3r. \quad (13.38)$$

Equation (13.36) is a matrix equation problem for the unknown $\beta_{L \rightarrow K}(\omega)$'s. To each electronic transition ($L \rightarrow K$) is associated an unknown $\beta_{L \rightarrow K}(\omega)$. This one may stress by the notational change $J \rightarrow I \equiv i$ and $L \rightarrow K \equiv j$. In the new notation, the set of equations in (13.36) takes the form

$$\beta_i(\omega) - \sum_j N_j^i(\omega) \beta_j(\omega) = H_i(\omega), \quad (13.39)$$

or equivalently

$$\sum_j (\delta_{ij} - N_j^i) \beta_j = H_i. \quad (13.40)$$

The reader should be cautious with the interpretation of the labeling in (13.39) and (13.40). Thus, the subscript j in N_j^i and β_j stands for $K \rightarrow L$ and $L \rightarrow K$, respectively, as it is apparent from (13.36). In the inhomogeneous set of linear equations among the unknown β_j 's, the column vector H_i depends on the external field only, cf. (13.38). The coefficients N_j^i are responsible for the electromagnetic coupling of the various electronic (many-body) transitions. Thus, it appears from (13.37) that the infinitesimal currents $\mathbf{J}_{J \rightarrow I}^T(\mathbf{r}) d^3r$ and $\mathbf{J}_{K \rightarrow L}^T(\mathbf{r}') d^3r'$ are coupled via the scalar propagator $g(|\mathbf{r} - \mathbf{r}'|; \omega)$. For a macroscopic object the number of relevant

electronic transitions will in general be extremely large, but for a mesoscopic (or microscopic) object the number of important transitions often will be quite limited. The dimension of the matrix N_j^i thus can be so small for a mesoscopic object that the local-field problem can be handled by numerical methods. However, it is also clear that a determination of the many-body energies and wave functions in itself constitutes a formidable problem even in the mesoscopic case. The calculation presented above for many-body dynamics fortunately can be carried out in an analogous manner for single-particle dynamics.

The determination of the local field by the method described above can also be used in near-field excitation studies where the transverse current density domains of the source and medium (mesoscopic, microscopic) overlap. In such cases the constitutive equation (13.26) must be replaced by the one in (12.119). Provided the response theory approximation still can be used one just needs to replace the external field appearing in (13.38) by the effective (eff) transverse driving field

$$\begin{aligned} E_T^{\text{eff}}(\mathbf{r}; \omega) &= E_T^{\text{ext}}(\mathbf{r}; \omega) \\ &+ i\mu_0\omega \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|; \omega) \mathbf{S}_{\text{TL}}(\mathbf{r}', \mathbf{r}''; \omega) \cdot \mathbf{E}_L^{\text{ext}}(\mathbf{r}''; \omega) d^3r'' d^3r'. \end{aligned} \quad (13.41)$$

After a brief discussion of local-field resonances in the subsequent subsection, the coupled-antenna theory presented above will be illustrated by a calculation of the transverse local field for a two-level system.

13.3.2 Local-Field Resonances

For a mesoscopic object (or a molecule or an atom) it is often possible to neglect the spatial variation of the transverse electric field across the object. In such cases, the expression for the quantity $\beta_{L \rightarrow K}(\omega)$, given in general by (13.33), is reduced to the form

$$\beta_{L \rightarrow K}(\omega) = \left[\int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^0(\mathbf{r}) d^3r \right] \cdot \mathbf{E}_T(\mathbf{0}; \omega), \quad (13.42)$$

assuming with no loss of generality that the mesoscopic object is located in the neighborhood of $\mathbf{r} = \mathbf{0}$. In view of (5.7) and (12.76), it appears that the integral in (13.42) is the (time independent) electric-dipole transition current density from state L to K . With the abbreviation

$$\mathbf{T}_T(\mathbf{r}; \omega) = \sum_{K, L} \mathbf{F}_{K \rightarrow L}^T(\mathbf{r}; \omega) \int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^0(\mathbf{r}) d^3r, \quad (13.43)$$

the transverse part of the local electric field at the space point $\mathbf{r}$ now is given by

$$\mathbf{E}_T(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + \mathbf{T}_T(\mathbf{r}; \omega) \cdot \mathbf{E}_T(\mathbf{0}; \omega). \quad (13.44)$$

The yet unknown local field $\mathbf{E}_T(\mathbf{0}; \omega)$ acting on the mesoscopic object is readily obtained setting $\mathbf{r} = \mathbf{0}$ in (13.44). The formal solution of the resulting equation is given by

$$\mathbf{E}_T(\mathbf{0}; \omega) = (\mathbf{U} - \mathbf{T}_T(\mathbf{0}; \omega))^{-1} \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{0}; \omega), \quad (13.45)$$

where $(\mathbf{U} - \mathbf{T}_T)^{-1}$ is the inverse matrix of $\mathbf{U} - \mathbf{T}_T$.

It is instructive at this point to compare the results in (13.44) and (13.45) to the classical analysis of the electrodynamic scattering from a single electric point-dipole. In Chap. 6, the electrodynamic interaction between electric point-dipoles was studied classically, and the difficulties associated to the incorporation of self-field effects were pointed out. In Sect. 7.2, we showed how a part of the self-field phenomenon, viz., the radiation damping could be incorporated on the basis of the nonrelativistic Abraham–Lorentz equation of motion. For an electric point-dipole, the radiation reaction manifests itself through the replacement of the bare ED-polarizability by a dressed polarizability. In the classical approach, the local electric field from a single electric point-dipole, located at the origo of the coordinate system, is given by (see (6.4) and (6.5))

$$\mathbf{E}(\mathbf{r}; \omega) = \mathbf{E}^{\text{ext}}(\mathbf{r}; \omega) + \mathbf{T}(\mathbf{r}; \omega) \cdot \mathbf{E}(\mathbf{0}; \omega), \quad (13.46)$$

where $\mathbf{T}(\mathbf{r}; \omega) = \mu_0 \omega^2 \mathbf{G}(\mathbf{r}; \omega) \cdot \boldsymbol{\alpha}(\omega)$, $\boldsymbol{\alpha}(\omega)$ being the dipole's polarizability tensor. The local field at the dipole site cannot be determined from this equation since the Green function $\mathbf{G}(\mathbf{r}; \omega)$, and consequently also $\mathbf{T}(\mathbf{r}; \omega)$, diverge for $\mathbf{r} \rightarrow \mathbf{0}$. The tensor $\mathbf{T}(\mathbf{r}; \omega)$ entering (13.44) does not diverge for $\mathbf{r} \rightarrow \mathbf{0}$, but takes on the finite value

$$\mathbf{T}_T(\mathbf{0}; \omega) = \sum_{K,L} A_{KL}(\omega) \left[\int_{-\infty}^{\infty} g(|\mathbf{r}|; \omega) \mathbf{J}_{K \rightarrow L}^T(\mathbf{r}) d^3 r \right] \left[\int_{-\infty}^{\infty} \mathbf{J}_{L \rightarrow K}^0(\mathbf{r}) d^3 r \right]. \quad (13.47)$$

In retrospect, it is the spatial nonlocal structure of the response tensor $\mathbf{S}_{TT}(\mathbf{r}, \mathbf{r}'; \omega)$, given by (13.27), which here has enabled us to obtain a finite value for the (transverse part of the) local electric field acting on the mesoscopic object.

In the approximation where $\beta_{L \rightarrow K}(\omega)$ is given by (13.42), selfsustaining local fields can exist at frequencies for which the resonance condition

$$\text{Det} \{ \mathbf{U} - \mathbf{T}_T(\mathbf{0}; \omega) \} = 0 \quad (13.48)$$

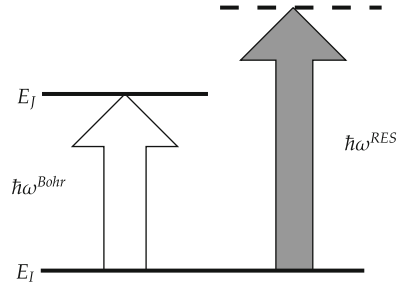
is satisfied. If the local-field corrections to the external field are sufficiently small the first-order Born approximation can be used to obtain

$$\mathbf{E}_T^{(1)}(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + \mathbf{T}_T(\mathbf{r}; \omega) \cdot \mathbf{E}_T^{\text{ext}}(\mathbf{0}; \omega), \quad (13.49)$$

cf. the discussion in Sect. 6.2. In this approximation, resonance occurs whenever the electronic (Bohr) resonance condition

$$\hbar \omega + E_L - E_K = 0 \quad (13.50)$$

Fig. 13.4 The presence of local-field effects displaces the electronic resonance frequency ω^{RES} slightly away from the Bohr frequency $\omega^{\text{Bohr}} = (E_J - E_I)/\hbar$ for the transition in consideration



is satisfied, provided irreversible damping mechanisms are neglected. In practice, the irreversible damping is always important near (at) resonance, and it prevents the field $\mathbf{E}_T^{(1)}(\mathbf{r}; \omega)$ from diverging at the Bohr resonance. Such a divergence would of course in itself invalidate any finite-order Born approximation calculations. In many cases, the various local-field resonance frequencies determined by (13.48) are only slightly displaced from the corresponding Bohr frequencies; see Fig. 13.4.

Even if one cannot assume that the transverse electric field is constant across the mesoscopic object it may still be possible to determine the position of the local-field resonances. Thus, it appears from (13.40) that the local-field resonance condition in the general case is given by

$$\text{Det} \{ \delta_{ij} - N_j^i(\omega) \} = 0. \quad (13.51)$$

For a given resonance (RES) frequency $\omega = \omega^{\text{RES}}$, the associated *relative* resonance values β_i^{RES} of the β_i 's are obtained from the homogeneous set of equations

$$\beta_i^{\text{RES}} - \sum_j N_j^i(\omega^{\text{RES}}) \beta_j^{\text{RES}} = 0. \quad (13.52)$$

To within an arbitrary constant the spatial form of the resonance field, $\mathbf{E}_T^{\text{RES}}(\mathbf{r}; \omega^{\text{RES}})$, finally can be determined from the equation

$$\mathbf{E}_T^{\text{RES}}(\mathbf{r}; \omega^{\text{RES}}) = \sum_{K,L} \mathbf{K}_{K \rightarrow L}^T(\mathbf{r}; \omega^{\text{RES}}) \beta_{L \rightarrow K}^{\text{RES}}, \quad (13.53)$$

cf. (13.34) with $\mathbf{E}_T^{\text{ext}} = \mathbf{0}$.

13.4 Two-Level System: Single Antenna Dynamics

It is instructive to apply the coupled-antenna formalism developed in the previous subsection to the case where only two energy levels, with energies E_1 and $E_2 (> E_1)$, say, play a significant role in the electrodynamic calculation. In general, a

mesoscopic (or microscopic) object cannot be considered as a two-level system, electronically. However, in cases where the electromagnetic frequency is close to the Bohr transition frequency, $(E_2 - E_1)/h$, and all other Bohr frequencies are far from this, roughly speaking, the two-level approximation may work well. It must be bared in mind that close to resonance, other things being equal, it is easier to drive the two-level system into the nonlinear regime, where the linear response theory, which forms the basis for the coupled antenna theory, fails [53, 178]. In the following the upwards and downwards transitions are denoted by the indices u and d , respectively, i.e., $1 \rightarrow 2 \equiv u$ and $2 \rightarrow 1 \equiv d$.

In the two-level approximation the local field, given in the general case by (13.34), takes the form

$$E_T(\mathbf{r}; \omega) = E_T^{\text{ext}}(\mathbf{r}; \omega) + \mathbf{F}_u^T(\mathbf{r}; \omega)\beta_d(\omega) + \mathbf{F}_d^T(\mathbf{r}; \omega)\beta_u(\omega). \quad (13.54)$$

It is physically appealing to consider the pair (1, 2) of states as equivalent to a single (microscopic) antenna from an electrodynamic point of view. Initially, the external field, $\mathbf{E}_T^{\text{ext}}(\mathbf{r}, t)$, induces a certain time dependent current density flow in the antenna. The flow distribution is a weighed superposition of the spatial forms of the transition current densities $\mathbf{J}_u$ and $\mathbf{J}_d$. The current density flow in turn give rise to emission of an electromagnetic field. The emitted field acts back on the antenna and changes its current density distribution, and thereafter the field emission. In the space–frequency domain the resulting (selfconsistent) local field is given by (13.54). Here, the field emissions in the up- and downwards transitions are proportional to $\mathbf{F}_u^T(\mathbf{r}; \omega)$ and $\mathbf{F}_d^T(\mathbf{r}; \omega)$. The amplitude strengths of these emissions are proportional to $\beta_d(\omega)$ and $\beta_u(\omega)$, respectively. Selfconsistency requires that

$$(1 - N_u^u)\beta_u - N_d^u\beta_d = H_u, \quad (13.55)$$

$$-N_u^d\beta_u + (1 - N_d^d)\beta_d = H_d, \quad (13.56)$$

cf. (13.40). From these equations one obtains

$$\beta_d = \frac{1}{D} \left[(1 - N_u^u)H_d + N_u^d H_u \right], \quad (13.57)$$

$$\beta_u = \frac{1}{D} \left[(1 - N_d^d)H_u + N_d^u H_d \right], \quad (13.58)$$

where

$$D = (1 - N_u^u)(1 - N_d^d) - N_u^d N_d^u \quad (13.59)$$

is the determinant of the set of equations. For the two-level system the resonance condition for the local field is given by

$$D(\omega^{\text{RES}}) = 0. \quad (13.60)$$

When the electromagnetic excitation frequency approaches the electronic transition frequency, it is often possible to use the so-called rotating-wave-approximation (RWA) [53, 178]. In this approximation the term containing $\mathbf{F}_u^T(\mathbf{r}; \omega)$ in (13.54) is neglected (the term has the nonresonant denominator $\hbar\omega + E_2 - E_1$ in A_{12}) (see (13.28) and (13.35)). The term $\mathbf{F}_d^T(\mathbf{r}; \omega)$ which is retained contains the resonant denominator $\hbar\omega + E_1 - E_2$. In the RWA model $\beta_d = 0$ implies that $\beta_u = H_u/(1 - N_u^u)$ (see (13.55)), so that one altogether obtains a local field

$$\mathbf{E}_T(\mathbf{r}; \omega) = \mathbf{E}_T^{\text{ext}}(\mathbf{r}; \omega) + \frac{H_u(\omega)}{1 - N_u^u(\omega)} \mathbf{F}_d^T(\mathbf{r}; \omega) \quad (13.61)$$

in this “simple” model.

Since a single pair of states in a sense is equivalent to a single microscopic antenna, it is understandable that a local-field theory which in a selfconsistent manner describes the electromagnetic interaction between (many) pairs of electronic energy levels may be called a coupled-antenna theory.

Chapter 14

Transverse and Covariant Electromagnetic Propagators: Principal Volume and Self-Field Dyadics

14.1 Transverse Propagator for the Electric Field

We have realized previously that the longitudinal part of the electric field can be eliminated as a dynamical variable in favour of the particle position coordinates. Such an elimination is particularly important in quantum mechanics where the canonical quantization scheme leads to the association of operators with the position coordinates. When the semiclassical theory of electrodynamics is extended to the quantum electrodynamic level in the Coulomb gauge certain operators are associated with the transverse degrees of freedom of the electromagnetic field. Via the quantization of the transverse part of the free electromagnetic field the photon concept is introduced. Since the photon necessarily propagates with the vacuum speed of light, it is of interest to seek to establish a propagator (Green function) description of the transverse field emission from a given microscopic current density distribution, $\mathbf{J}(\mathbf{r}, t)$. The work towards this goal makes clear the particular importance of the rim zone for the particle-field interaction.

14.1.1 Spectral Representation

In Chap. 3, we introduced in the space–frequency domain a dyadic Green function $\mathbf{G}(\mathbf{R}; \omega)$ for the electric field (3.22). For points outside the domain of the microscopic current density distribution $\mathbf{J}(\mathbf{r}; \omega)$ this Green function enters the integral relation between the *total* microscopic electric field $\mathbf{E}(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$; see (3.21) and (3.23). By means of the scalar propagator $g(\mathbf{R}; \omega)$ an integral relation between the *transverse* parts of the electric field ($\mathbf{E}_T(\mathbf{r}; \omega)$) and current density ($\mathbf{J}_T(\mathbf{r}; \omega)$) was established in Chap. 13, and it appeared from our analysis that the integral relation (13.25) also holds everywhere inside the domain of the transverse current density. Below we shall see how a propagator $\mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega)$ relating the *transverse part* of the electric field at point $\mathbf{r}$ to the *total* current density at point $\mathbf{r}'$ can be introduced. For the time being it will be assumed that the two points do not coincide, i.e., $\mathbf{R} = \mathbf{r} - \mathbf{r}' \neq \mathbf{0}$.

It appears from (9.27) that the longitudinal parts of the electric field and current density are related by the spatially local equation

$$\mathbf{E}_L(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \mathbf{J}_L(\mathbf{r}; \omega) \quad (14.1)$$

in the spectral representation. Formally, $\mathbf{E}_L(\mathbf{r}; \omega)$ can in turn be related to the total current density by means of the longitudinal delta function; see (9.18). Hence, one obtains the spatially nonlocal connection

$$\mathbf{E}_L(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \int_{-\infty}^{\infty} \delta_L(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r'. \quad (14.2)$$

In spherical contraction, $\delta_L(\mathbf{R})$ is given by (9.20), but for field points outside the current density distribution ($\mathbf{R} \neq \mathbf{0}$) the local part $U\delta(\mathbf{R})/3$ is absent, and there thus is no need for a contraction procedure since the integrand has no singularity. With reference to the general vector field relation in (9.7) one may safely interchange the integral and double differential $(-\nabla\nabla\cdot)$ operations for $\mathbf{r} \neq \mathbf{r}'$ that is

$$\begin{aligned} \mathbf{W}_L(\mathbf{r}) &= \int_{-\infty}^{\infty} (-\nabla)\nabla \cdot \left(\frac{\mathbf{W}(\mathbf{r}')}{4\pi|\mathbf{r} - \mathbf{r}'|} \right) d^3r' \\ &= \int_{-\infty}^{\infty} \left[-\nabla\nabla \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} \right] \cdot \mathbf{W}(\mathbf{r}') d^3r', \quad \mathbf{r} \neq \mathbf{r}'. \end{aligned} \quad (14.3)$$

In view of (14.3), (14.2) can be written in the form

$$\mathbf{E}_L(\mathbf{r}; \omega) = i\mu_0\omega \int_{-\infty}^{\infty} \left[\frac{1}{q_0^2} \nabla\nabla \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} \right] \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r', \quad (14.4)$$

or equivalently as

$$\mathbf{E}_L(\mathbf{r}; \omega) = i\mu_0\omega \int_{-\infty}^{\infty} [q_0^{-2} \nabla\nabla g(|\mathbf{r} - \mathbf{r}'|; 0)] \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r', \quad (14.5)$$

where $g(R; 0) = (4\pi R)^{-1}$ is the Huygens propagator in the limit $q_0 \rightarrow 0$. By subtracting (14.5) from (3.21) one obtains

$$\mathbf{E}_T(\mathbf{r}; \omega) = i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r', \quad \mathbf{r} \neq \mathbf{r}', \quad (14.6)$$

where

$$\begin{aligned} \mathbf{G}_T(\mathbf{R}; \omega) &= \mathbf{G}(\mathbf{R}; \omega) - q_0^{-2} \nabla\nabla g(R; 0) \\ &= U g(R; \omega) + q_0^{-2} \nabla\nabla (g(R; \omega) - g(R; 0)). \end{aligned} \quad (14.7)$$

The dyadic Green function $\mathbf{G}_T(\mathbf{R}; \omega)$ being the sought for kernel in the integral relation between $\mathbf{E}_T(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$ commonly is called the *transverse propagator* (for the electric field). Obviously, $\mathbf{G}_T(\mathbf{R}; \omega)$ is a symmetric tensor. Since

$$\nabla \nabla g(R; 0) = \frac{3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U}}{4\pi R^3}, \quad (14.8)$$

as expected in view of (9.18), (9.20) and (14.4), (3.32) and (14.7) show that one may write the transverse propagator in the explicit form

$$\mathbf{G}_T(\mathbf{R}; \omega) = \frac{iq_0}{4\pi} \left\{ \frac{e^{iq_0 R}}{iq_0 R} (\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}) - \left[\frac{e^{iq_0 R}}{(iq_0 R)^2} - \frac{e^{iq_0 R} - 1}{(iq_0 R)^3} \right] (\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) \right\}. \quad (14.9)$$

The dyadic Green function for the magnetic field, also called the transverse propagator for the magnetic field, is related to $\mathbf{G}_T(\mathbf{R}; \omega)$ as follows

$$\mathbf{G}_M(\mathbf{R}; \omega) = (iq_0)^{-1} \nabla \times \mathbf{G}_T(\mathbf{R}; \omega). \quad (14.10)$$

This result follows readily from (3.28), and the fact that $\nabla \times \nabla \nabla g(R, 0) = \mathbf{0}$. This must be so of course since the magnetic field is a transverse vector field.

14.1.2 Genuine Transversality

Although the total electric field according to the Maxwell equation in (3.6) is divergence-free ($\nabla \cdot \mathbf{E}(\mathbf{r}; \omega) = 0$) in vacuum, and (3.21), therefore, immediately shows that the divergence of the standard Green function $\mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega)$ vanishes for $\mathbf{r} \neq \mathbf{r}'$, i.e.,

$$\nabla \cdot \mathbf{G}(\mathbf{R}; \omega) = \mathbf{0}, \quad \mathbf{R} \neq \mathbf{0}, \quad (14.11)$$

one cannot conclude that $\mathbf{G}(\mathbf{R}; \omega)$ is a *genuine* transverse dyadics, because to qualify as such also the role of the singular point at $\mathbf{R} = \mathbf{0}$ must be investigated, cf. the discussion in Sect. 9.1. As we shall realize below the singularity does affect the standard Green function in the limit $\mathbf{R} \rightarrow \mathbf{0}$. Since $\nabla \cdot \mathbf{E}_T(\mathbf{r}; \omega) = 0$ everywhere in space per definition, (14.6) allows one to conclude that

$$\nabla \cdot \mathbf{G}_T(\mathbf{R}; \omega) = \mathbf{0}, \quad \mathbf{R} \neq \mathbf{0} \quad (14.12)$$

Let us now prove that $\mathbf{G}_T(\mathbf{R}; \omega)$ is a genuine transverse dyadic quantity, and that $\mathbf{G}(\mathbf{R}; \omega)$ is not. For this purpose it is useful to say a few words about the singular differential equation for the scalar propagator (3.42). Since $\nabla = \nabla_R$, where ∇_R is the gradient with respect to $\mathbf{R}$, integration of the first term on the left side of (3.42) over a sphere centered on $R = 0$ and of radius ϵ gives in view of Gauss' theorem

$$\int_{R=\epsilon}^{\epsilon} \nabla_R^2 g(R; \omega) d^3 R = \oint_{R=\epsilon} \hat{\mathbf{R}} \cdot \nabla_R g(R; \omega) dS = (iq_0 \epsilon - 1) e^{iq_0 \epsilon}. \quad (14.13)$$

In the limit $\epsilon \rightarrow 0$, the integral in (14.13) thus equals -1 . The integral of the second term in (3.42) vanishes in this limit:

$$\lim_{\epsilon \rightarrow 0} \left\{ q_0^2 \int^\epsilon 4\pi R^2 g(R; \omega) dR \right\} = q_0^2 \lim_{\epsilon \rightarrow 0} \int_0^\epsilon R dR = 0. \quad (14.14)$$

The integration of $-\delta(\mathbf{R})$ over a volume containing the point $\mathbf{R} = \mathbf{0}$ gives -1 , and it therefore appears that the necessity of the presence of the delta function in (3.42) originates in the fact that the volume integral of $\nabla_R^2 g(\mathbf{R}; \omega)$ is -1 . Hence, it is because of the double nabla operation ($\nabla \cdot \nabla$) that the delta function affects the solution of the differential equation for the scalar propagator in points outside the singularity. The Green functions $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_T(\mathbf{R}; \omega)$ contain double nabla operations ($\nabla \nabla$) on the scalar propagator $g(\mathbf{R}; \omega)$, and on the difference $g(\mathbf{R}; \omega) - g(\mathbf{R}; 0)$, respectively, see (14.7). These operations affect the divergences of the Green functions differently. Thus, one obtains from (3.22) and (3.42), and $\nabla \cdot (g\mathbf{U}) = \nabla g$,

$$\nabla \cdot \mathbf{G}(\mathbf{R}; \omega) = q_0^{-2} \nabla [(\nabla^2 + q_0^2)g(\mathbf{R}; \omega)] = -q_0^{-2} \delta(\mathbf{R}). \quad (14.15)$$

The Green function $\mathbf{G}(\mathbf{R}; \omega)$ therefore does not qualify as a *genuine* transverse dyadic quantity, because its divergence does not vanish in $\mathbf{R} = \mathbf{0}$. For $\mathbf{G}_T(\mathbf{R}; \omega)$, on the other hand, one finds for *all* $\mathbf{R}$

$$\nabla \cdot \mathbf{G}_T(\mathbf{R}; \omega) = q_0^{-2} \nabla [(\nabla^2 + q_0^2)g(\mathbf{R}; \omega) - \nabla^2 g(\mathbf{R}; 0)] = 0, \quad (14.16)$$

since $\nabla^2 g(\mathbf{R}; 0) = -\delta(\mathbf{R})$. The transverse propagator thus qualifies as a *genuine* transverse dyad.

14.1.3 Space–Time Form: Causality and Space-Like Near-Field Coupling

In Chap. 3, we studied the standard Green function for the electric field in the spectral representation in some detail. *All* our considerations in that chapter referred to this representation, and the reader may have wondered already then why we did not transform the propagator from the mixed space–frequency domain to the space–time domain. Above all, the space–time description of electrodynamics plays a particularly direct physical role, and the standard Green function has been used time and time again in theoretical investigations in near-field optics. There is a very good reason for our use of the spectral representation: The standard Green function $\mathbf{G}$ does not exist in the space–time domain! In textbooks, this fact is never pointed out, and many authors apparently believe that a straightforward timely Fourier transformation of $\mathbf{G}(\mathbf{R}; \omega)$ will provide us with a space–time representative of the standard Green function for the electric field. Many authors use the word *propagator* instead of the words *Green function* for $\mathbf{G}(\mathbf{R}; \omega)$, and I have done this

myself on previous occasions, sometimes. Literally, the word *propagator* refers to propagation, and propagation (of electromagnetic fields) must refer to space–time dynamics. In this book, we shall distinguish between “Green function” and “propagator.” The reason that the standard propagator $\mathbf{G}(\mathbf{R}; \omega)$, given in adequate closed form in (3.32), cannot be transformed to the space–time domain can be traced back to the fact that its near-field part $\mathbf{G}^{\text{NF}}(\mathbf{R}; \omega)$ (3.40) has a frequency dependence of the form $\omega^{-2} \exp(i \frac{R}{c_0} \omega)$, and the Fourier transform of this type of function does not exist, as the reader may convince herself of. Although the standard Green function for the electric field does not exist in the space–time domain this *does not* imply that the integral relation between the electric field, $\mathbf{E}(\mathbf{r}; \omega)$, and current density, $\mathbf{J}(\mathbf{r}; \omega)$, given in (3.21), cannot be transformed to this domain. Thus, when the near-field part of $\mathbf{G}(\mathbf{R}; \omega)$ is multiplied by the ω -factor in front of the integral in (3.21) one obtains a functional form $\omega^{-1} \exp(i \frac{R}{c_0} \omega)$ which Fourier transform *does* exist. Since the elementary quantum excitations of the free electromagnetic field, the photons, *propagate* through space (with the speed c_0), one would expect that a genuine physical photon propagator exists in the space–time domain. Since the photons are related to the transverse part of the electromagnetic field, and the integral relation between $\mathbf{E}_T(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$ involves the transverse propagator $\mathbf{G}_T(\mathbf{R}; \omega)$ (note the name!) one perhaps would expect beforehand that the transverse propagator does have a space–time representative. A comparison of (3.32) and (14.9) shows that the near-field part $\omega^{-2} \exp(i \frac{R}{c_0} \omega)$ of $\mathbf{G}(\mathbf{R}; \omega)$ is replaced by a part $\omega^{-2} [\exp(i \frac{R}{c_0} \omega) - 1]$ in $\mathbf{G}_T(\mathbf{R}; \omega)$. The presence of this extra -1 in the nominator has the consequence that the transverse propagator $\mathbf{G}_T(\mathbf{R}; \omega)$ *can* be transformed to the space–time domain, as we shall see below. Physically, the extra -1 originates in the subtraction of the nonpropagating longitudinal electric field from the total field, cf. the description in Sect. 14.1.1. Before proceeding let me emphasize that above all it is for near-field electrodynamics the distinction between $\mathbf{G}$ and $\mathbf{G}_T$ becomes of crucial importance.

Before presenting the final expression for the space–time representative $\mathbf{G}_T(\mathbf{R}, \tau)$ of the transverse propagator, it is instructive to examine the timely Fourier transforms of the far-, mid- and near-field parts of the $\mathbf{G}_T(\mathbf{R}, \omega)$ in (14.9), separately. The far-field part is proportional to

$$I_{\text{FF}} \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\frac{R}{c_0} - \tau)\omega} d\omega = \delta(\frac{R}{c_0} - \tau), \quad (14.17)$$

and is, therefore, as one might have expected, only nonvanishing on the light cone. Explicitly, one obtains

$$\mathbf{G}_T^{\text{FF}}(\mathbf{R}, \tau) = \frac{1}{4\pi R} \delta(\frac{R}{c_0} - \tau) (\mathbf{U} - \hat{\mathbf{R}} \hat{\mathbf{R}}). \quad (14.18)$$

The factor in front of $\mathbf{U} - \hat{\mathbf{R}} \hat{\mathbf{R}}$ is just the retarded scalar propagator (2.18). In the radiation zone one of course has

$$\mathbf{G}_T^{\text{FF}}(\mathbf{R}, \tau) = \mathbf{G}^{\text{FF}}(\mathbf{R}, \tau). \quad (14.19)$$

The transform of the mid-field part of $\mathbf{G}_T(\mathbf{R}; \omega)$ is proportional to

$$\begin{aligned} I_{\text{MF}} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(\frac{R}{c_0} - \tau)\omega} \frac{d\omega}{\omega} = \frac{i}{2\pi} \int_{-\infty}^{\infty} \sin\left(\frac{R}{c_0} - \tau\right) \frac{d\omega}{\omega} \\ &= \frac{i}{2} \text{sgn}\left(\frac{R}{c_0} - \tau\right). \end{aligned} \quad (14.20)$$

The last equality in (14.20) is obtained by use of the well-known formula

$$\int_{-\infty}^{\infty} \frac{\sin(mx)}{x} dx = \pi \text{sgn}(m). \quad (14.21)$$

Altogether, the mid-field part of the transverse propagator becomes

$$\mathbf{G}_T^{\text{MF}}(\mathbf{R}, \tau) = \frac{c_0}{8\pi R^2} \text{sgn}\left(\tau - \frac{R}{c_0}\right) (\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}). \quad (14.22)$$

The mid-field part of $\mathbf{G}_T(\mathbf{R}, \tau)$ is noncausal since it does not vanish for $\tau < 0$. This is not fatal physically because only the sum of the mid- and near-field parts of the transverse propagator plays a physical role. We shall realize below that this sum obeys the causality demand. Equation (14.22) displays another at first sight unphysical feature in that $\mathbf{G}_T^{\text{MF}}(\mathbf{R}, \tau)$ is nonvanishing in front of the light cone, i.e., for $\tau < R/c_0$. This space-like coupling of $\mathbf{E}_T$ and $\mathbf{J}$ is *not* canceled when the near-field part of the transverse propagator is added. As we shall realize, there is a satisfactory explanation for this seemingly unphysical result. The propagation characteristics of $\mathbf{G}_T^{\text{MF}}(\mathbf{R}, \tau)$ is related only to the sign reversal point of the signum function. Sign reversal appears for $\tau = R/c_0$, and the spherical surface defined by this relation moves outwards from $R = 0$ with the vacuum speed of light.

The near-field part of $\mathbf{G}_T(\mathbf{R}, \tau)$ has a Fourier transform proportional to

$$\begin{aligned} I_{\text{NF}} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(e^{i\frac{R}{c_0}\omega} - 1 \right) e^{-i\omega\tau} \frac{d\omega}{\omega^2} \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} (1 - e^{-i\omega\tau}) \frac{d\omega}{\omega^2} - \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[1 - e^{i(\frac{R}{c_0} - \tau)\omega} \right] \frac{d\omega}{\omega^2} \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} (1 - \cos \omega\tau) \frac{d\omega}{\omega^2} - \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[1 - \cos\left(\frac{R}{c_0} - \tau\right)\omega \right] \frac{d\omega}{\omega^2}. \end{aligned} \quad (14.23)$$

With the help of the formula

$$\int_{-\infty}^{\infty} (1 - \cos mx) \frac{dx}{x^2} = \pi |m| \quad (14.24)$$

one thus obtains

$$I_{\text{NF}} = \frac{1}{2} \left(|\tau| - \left| \frac{R}{c_0} - \tau \right| \right), \quad (14.25)$$

and finally after some algebraic manipulations

$$\mathbf{G}_T^{\text{NF}}(\mathbf{R}, \tau) = \frac{c_0^2}{8\pi R^3} \left(\left| \frac{R}{c_0} - \tau \right| - |\tau| \right) \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} \right). \quad (14.26)$$

As it was the case with the mid-field part of the transverse propagator, the near-field part is (1) noncausal (nonvanishing for $\tau < 0$) and (2) nonvanishing in front of the light cone. The mid- and near-field parts are both nonvanishing behind the light cone, but the sum does not connect time-like events, as we shall see. This, at first sight seemingly unphysical result is satisfactory, however.

By addition of (14.22) and (14.26) one obtains

$$\mathbf{G}_T^{\text{MF}}(\mathbf{R}, \tau) + \mathbf{G}_T^{\text{NF}}(\mathbf{R}, \tau) = \frac{c_0}{8\pi R^2} f(R, \tau) \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} \right), \quad (14.27)$$

where

$$f(R, \tau) = \text{sgn} \left(\tau - \frac{R}{c_0} \right) + \frac{c_0}{R} \left(\left| \frac{R}{c_0} - \tau \right| - |\tau| \right). \quad (14.28)$$

Simple considerations show that $f(R, \tau)$ can be written in the form

$$f(R, \tau) = -\frac{2c_0\tau}{4\pi R^3} \theta(\tau) \theta \left(\frac{R}{c_0} - \tau \right), \quad (14.29)$$

and when (14.29) is inserted into (14.27) one gets

$$\mathbf{G}_T^{\text{MF}}(\mathbf{R}, \tau) + \mathbf{G}_T^{\text{NF}}(\mathbf{R}, \tau) = -\frac{c_0^2\tau}{4\pi R^3} \theta(\tau) \theta \left(\frac{R}{c_0} - \tau \right) \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} \right). \quad (14.30)$$

Let us now dwell for a moment on the physical interpretation of the result in (14.30). The step function $\theta(\tau)$ ensures that the sum of the mid- and near-field contributions is causal, a satisfactory physical result. The presence of the step function $\theta(\frac{R}{c_0} - \tau)$ tells us that the sum *only* connects $\mathbf{E}_T(\mathbf{r}, t)$ and $\partial \mathbf{J}(\mathbf{r}', t')/\partial t'$ in a space-like manner. In itself, this is *not* in conflict with Einsteinian causality. To understand this, the reader should remember that one arrives at

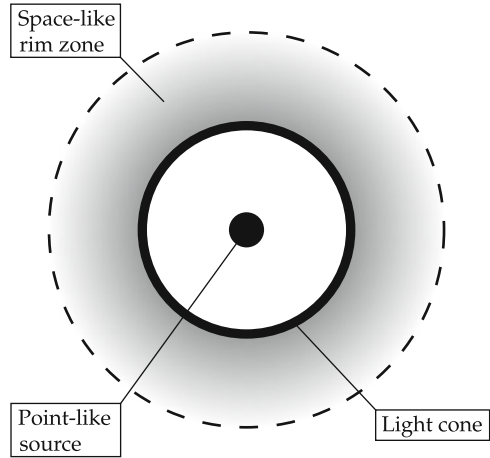
$$\mathbf{E}_T(\mathbf{r}, t) = -\mu_0 \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{R}, \tau) \cdot \frac{\partial}{\partial t'} \mathbf{J}(\mathbf{r}', t') d^3 r' dt', \quad (14.31)$$

starting from

$$\mathbf{E}_T(\mathbf{r}, t) = -\mu_0 \int_{-\infty}^{\infty} g(R, \tau) \frac{\partial}{\partial t'} \mathbf{J}_T(\mathbf{r}', t') d^3 r' dt'. \quad (14.32)$$

(Equation (14.31) is the timely Fourier transform of (14.6), and (14.32) is the integral part of (10.4)). The Huygens propagator in (14.32) is nonvanishing only on the light cone and (14.32) therefore connects $\mathbf{E}_T(\mathbf{r}, t)$ and $\partial \mathbf{J}_T(\mathbf{r}', t')/\partial t'$ in an

Fig. 14.1 Rim-zone radiation from a point-like source in space–time. The near-field part of the transverse propagator is nonvanishing only in front of the light cone. The space-like part of the rim zone is indicated in a light grey tone. The space-like nonlocality originates in the circumstance that the extension of the rim zone corresponds to the best spatial localization achievable for a photon field



Einstein causal manner. When the source domain “artificially” is compressed from $\mathbf{J}_T$ to $\mathbf{J}$, when replacing (14.32) by (14.31), space-like couplings necessarily must occur in the formalism since this compression is carried out with the help of the transverse delta function, a time independent dyadic. Hence,

$$\mathbf{G}_T(\mathbf{r} - \mathbf{r}', \tau) = \int_{-\infty}^{\infty} g(\mathbf{r} - \mathbf{r}'', \tau) \delta_T(\mathbf{r}'' - \mathbf{r}') d^3 r''. \quad (14.33)$$

Time-like couplings are absent in (14.30), and this fact makes the result particularly beautiful: For *finite* $\tau (> 0)$ the sum of mid-field- and near-field-parts of the transverse propagator is zero behind the light cone [$\theta(R/c_0 - \tau) = 0$ for $\tau > R/c_0$], and the right side of (14.30), therefore, is nonsingular for fixed but finite $\tau (> 0)$.

By adding (14.18) and (14.30) it appears that the transverse propagator for the electric field takes the following form in the space–time domain:

$$\begin{aligned} \mathbf{G}_T(\mathbf{R}, \tau) = & \frac{1}{4\pi R} \delta\left(\frac{R}{c_0} - \tau\right) (\mathbf{U} - \hat{\mathbf{R}}\hat{\mathbf{R}}) \\ & - \frac{c_0^2 \tau}{4\pi R^3} \theta(\tau) \theta\left(\frac{R}{c_0} - \tau\right) (\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}). \end{aligned} \quad (14.34)$$

It is remarkable that the transverse propagator in the space–time domain has no mid-field part, only a far-field (R^{-1}) light-cone part plus a near-field (R^{-3}) space-like part. The near-field part of $\mathbf{G}_T(\mathbf{R}, \tau)$ increases linearly in time (τ) in every space point until the time when the light cone sweeps across the given point. Thereafter, the near-field part of the propagator vanishes, as illustrated in Fig. 14.1.

14.2 Eigenvector Expansion of Propagators

14.2.1 Distribution Theory

In the framework of distribution theory, the scalar propagator satisfies the inhomogeneous wave equation (3.42). The delta-function singularity is responsible for the presence of the normalization factor $(4\pi)^{-1}$ by which the function $\exp(iq_0 R)/R$ is multiplied to give the scalar propagator. This is the only effect of the Dirac delta function. The standard Green function for the electric field satisfies the differential equation (3.46), or equivalently

$$-\nabla \times (\nabla \times \mathbf{G}^{\text{gen}}(\mathbf{R}; \omega)) + q_0^2 \mathbf{G}^{\text{gen}}(\mathbf{R}; \omega) = -\delta(\mathbf{R})\mathbf{U}, \quad (14.35)$$

in a notation where a superscript *gen* (standing for generalized) has been added to $\mathbf{G}(\mathbf{R}; \omega)$. The reason for this addition is due to the fact that the effect of the delta-function singularity not just manifests itself as a normalization factor on the solution for $\mathbf{R} \neq \mathbf{0}$. In consistency with our previous notation, the name $\mathbf{G}(\mathbf{R}; \omega)$ is reserved for the solution to (14.35) for $\mathbf{R} \neq \mathbf{0}$, cf. (3.22). The propagators $\mathbf{G}^{\text{gen}}(\mathbf{R}; \omega)$ and $\mathbf{G}(\mathbf{R}; \omega)$ deviate from each other by a dyadic function which is singular at the point $\mathbf{R} = \mathbf{0}$, as we shall see later on.

By division of the Green function $\mathbf{G}^{\text{gen}}$ into its transverse ($\mathbf{G}_T^{\text{gen}}$) and longitudinal ($\mathbf{G}_L^{\text{gen}}$) parts, i.e.,

$$\mathbf{G}^{\text{gen}}(\mathbf{R}; \omega) = \mathbf{G}_T^{\text{gen}}(\mathbf{R}; \omega) + \mathbf{G}_L^{\text{gen}}(\mathbf{R}; \omega), \quad (14.36)$$

where

$$\nabla \cdot \mathbf{G}_T^{\text{gen}}(\mathbf{R}; \omega) = \mathbf{0}, \quad (14.37)$$

$$\nabla \times \mathbf{G}_L^{\text{gen}}(\mathbf{R}; \omega) = \mathbf{0}, \quad (14.38)$$

and by use of the delta-function division in (9.21), it follows that (14.35) can be split into the two equations

$$(\nabla^2 + q_0^2)\mathbf{G}_T^{\text{gen}}(\mathbf{R}; \omega) = -\delta_T(\mathbf{R}), \quad (14.39)$$

and

$$q_0^2 \mathbf{G}_L^{\text{gen}}(\mathbf{R}; \omega) = -\delta_L(\mathbf{R}). \quad (14.40)$$

The solution of (14.40) will be denoted by $\mathbf{g}_L(\mathbf{R}; \omega)$ and given the name *the longitudinal self-field propagator*. From time to time $\mathbf{g}_L(\mathbf{R}; \omega)$ also will be called *the longitudinal source dyadic*. It immediately appears from (14.40) that

$$\mathbf{g}_L^{\text{gen}}(\mathbf{R}; \omega) = -q_0^{-2} \delta_L(\mathbf{R}). \quad (14.41)$$

The proportionality of $\mathbf{g}_L$ and δ_L makes it clear that one cannot give an explicit expression for the longitudinal self-field propagator unless the form of the

contraction volume is specified. In spherical contraction $\delta_L(\mathbf{R})$ is given by (9.20). Since

$$\mathbf{G}_T^{\text{gen}}(\mathbf{R}; \omega) = \mathbf{G}_T(\mathbf{R}; \omega), \quad \mathbf{R} \neq \mathbf{0}, \quad (14.42)$$

the transverse propagator $\mathbf{G}_T(\mathbf{R}; \omega)$ must satisfy (14.39) everywhere in space except at $\mathbf{R} = \mathbf{0}$, where it is not defined. One may verify that this is correct by working with the operator on the last expression in (14.7). After interchange of the $\nabla^2 + q_0^2$ and $\nabla\nabla$ operations, and use of (3.42) for $\mathbf{r} \neq \mathbf{r}'$, one obtains

$$(\nabla^2 + q_0^2)\mathbf{G}_T(\mathbf{R}; \omega) = -q_0^{-2}\nabla\nabla[(\nabla^2 + q_0^2)g(\mathbf{R}; 0)]. \quad (14.43)$$

In the limit $\omega \rightarrow 0$, (3.42) immediately gives

$$\nabla^2 g(\mathbf{R}; 0) = 0 \quad (14.44)$$

for $\mathbf{R} \neq \mathbf{0}$, and hence via (9.19) and (14.8)

$$(\nabla^2 + q_0^2)\mathbf{G}_T(\mathbf{R}; \omega) = -\nabla\nabla g(\mathbf{R}; 0) = -\delta_T(\mathbf{R}), \quad \mathbf{R} \neq \mathbf{0}, \quad (14.45)$$

which is just the differential equation in (14.39) for the generalized transverse propagator outside the singularity.

14.2.2 Transverse Eigenvector Expansion over a Finite Domain

Let us now briefly consider solutions ($\boldsymbol{\eta}^T$) to the vectorial Helmholtz equation

$$(\nabla^2 + q^2)\boldsymbol{\eta}^T(\mathbf{r}) = \mathbf{0}, \quad (14.46)$$

which satisfy the transversality condition $\nabla \cdot \boldsymbol{\eta}^T(\mathbf{r}) = 0$. If the solutions are required to satisfy appropriate boundary conditions [289] on the surface of the volume of interest, Ω , (14.46) will in general only have acceptable solutions for certain values of q , called the eigenvalues. For a finite domain the spectrum of eigenvalues is a discrete set, and we denote the eigenvalues by q_n . The transverse eigenfunction belonging to q_n is denoted by $\boldsymbol{\eta}_n^T$. The eigenvalue differential equation for index n thus reads

$$(\nabla^2 + q_n^2)\boldsymbol{\eta}_n^T(\mathbf{r}) = \mathbf{0}. \quad (14.47)$$

The eigenfunctions belonging to different n 's can be shown to be orthogonal, and can be assumed to be normalized. Over the Ω domain the eigenvectors hence obey the orthonormality condition

$$\int_{\Omega} (\boldsymbol{\eta}_m^T(\mathbf{r}))^* \cdot \boldsymbol{\eta}_n^T(\mathbf{r}) d^3r = \delta_{mn}, \quad (14.48)$$

and it is assumed that the totality of eigenfunctions form a complete set. The completeness is expressed through the completeness theorem for the transverse spectrum, viz.,

$$\sum_n \boldsymbol{\eta}_n^T(\mathbf{r})(\boldsymbol{\eta}_n^T(\mathbf{r}_0))^* = \boldsymbol{\delta}_T(\mathbf{r} - \mathbf{r}_0). \quad (14.49)$$

If one assumes that the transverse Green function dyadic for the finite Ω domain, denoted by $\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0; \omega)$, and satisfying

$$(\nabla^2 + q_0^2)\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0; \omega) = -\boldsymbol{\delta}_T(\mathbf{r} - \mathbf{r}_0), \quad (14.50)$$

has the same boundary conditions as the eigenfunctions, then this Green function can be expanded in a series of the eigenfunctions $\boldsymbol{\eta}_n^T$. To show this, let us first write $\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0; \omega) \equiv \boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0)$ in the form

$$\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0) = \sum_{\substack{i,j= \\ x,y,z}} \Gamma_{T,ij}(\mathbf{r}, \mathbf{r}_0) \hat{\mathbf{e}}_i \hat{\mathbf{e}}_j, \quad (14.51)$$

where $\hat{\mathbf{e}}_i$ ($\hat{\mathbf{e}}_j$) is a unit vector along the Cartesian axis i (j). By means of the function

$$\mathbf{F}_j(\mathbf{r}, \mathbf{r}_0) \equiv \sum_i \Gamma_{T,ij}(\mathbf{r}, \mathbf{r}_0) \hat{\mathbf{e}}_i, \quad (14.52)$$

Equation (14.51) can also be written as follows:

$$\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0) = \sum_j \mathbf{F}_j(\mathbf{r}, \mathbf{r}_0) \hat{\mathbf{e}}_j. \quad (14.53)$$

Next, $\mathbf{F}_j(\mathbf{r}, \mathbf{r}_0)$ is expanded in terms of the complete set $\{\boldsymbol{\eta}_n^T(\mathbf{r})\}$, i.e.,

$$\mathbf{F}_j(\mathbf{r}, \mathbf{r}_0) = \sum_m A_m^j(\mathbf{r}_0) \boldsymbol{\eta}_m^T(\mathbf{r}), \quad (14.54)$$

where the expansion coefficients $A_m^j(\mathbf{r}_0)$ are functions of $\mathbf{r}_0$. By inserting (14.54) into (14.53) one obtains

$$\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0) = \sum_{j,m} A_m^j(\mathbf{r}_0) \boldsymbol{\eta}_m^T(\mathbf{r}) \hat{\mathbf{e}}_j, \quad (14.55)$$

and then with the use of the eigenvalue equation in (14.47)

$$\nabla^2 \boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0) = - \sum_{j,m} q_m^2 A_m^j(\mathbf{r}_0) \boldsymbol{\eta}_m^T(\mathbf{r}) \hat{\mathbf{e}}_j. \quad (14.56)$$

By combining (14.50), (14.55), and (14.56) one gets

$$\sum_{j,m} (q_0^2 - q_m^2) A_m^j(\mathbf{r}_0) \boldsymbol{\eta}_m^T(\mathbf{r}) \hat{\mathbf{e}}_j = -\delta_T(\mathbf{r} - \mathbf{r}_0). \quad (14.57)$$

A scalar multiplication of (14.57) by $(\boldsymbol{\eta}_n^T(\mathbf{r}))^*$ from the left, followed by an integration over the Ω domain gives

$$\begin{aligned} \sum_{j,m} (q_0^2 - q_m^2) A_m^j(\mathbf{r}_0) \left[\int^\Omega (\boldsymbol{\eta}_n^T(\mathbf{r}))^* \cdot \boldsymbol{\eta}_m^T(\mathbf{r}) d^3r \right] \hat{\mathbf{e}}_j \\ = - \int^\Omega (\boldsymbol{\eta}_n^T(\mathbf{r}))^* \cdot \delta_T(\mathbf{r} - \mathbf{r}_0) d^3r. \end{aligned} \quad (14.58)$$

The orthonormality of the transverse eigenvectors over the Ω domain (14.48), and the definition of the transverse delta function, simplify (14.58) to

$$\sum_j (q_0^2 - q_n^2) A_n^j(\mathbf{r}_0) \hat{\mathbf{e}}_j = -(\boldsymbol{\eta}_n^T(\mathbf{r}_0))^*, \quad (14.59)$$

or equivalently

$$\sum_j A_n^j(\mathbf{r}_0) \hat{\mathbf{e}}_j = \frac{(\boldsymbol{\eta}_n^T(\mathbf{r}_0))^*}{q_n^2 - q_0^2}. \quad (14.60)$$

The eigenvector expansion of the Green function finally is obtained by inserting (14.60) into (14.55). Thus, with the index change $m \rightarrow n$ in (14.54), one arrives at the following result

$$\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0; \omega) = \sum_n \frac{\boldsymbol{\eta}_n^T(\mathbf{r})(\boldsymbol{\eta}_n^T(\mathbf{r}_0))^*}{q_n^2 - q_0^2}. \quad (14.61)$$

Viewed as a function of q_0 , $\boldsymbol{\Gamma}_T(\mathbf{r}, \mathbf{r}_0; \omega)$ has poles at each eigenvalue q_n of q_0 .

14.2.3 Plane-Wave Eigenvector Expansion Over an Infinite Domain

Particularly useful expressions can be obtained for $\boldsymbol{G}_T(\mathbf{r} - \mathbf{r}_0; \omega)$ and $\boldsymbol{g}_L(\mathbf{r} - \mathbf{r}_0; \omega)$ if plane-wave eigenvector expansions over an infinite domain is employed. Thus, associated with each wave vector $\mathbf{q}$ one introduces two transversely polarized and linearly independent eigenvectors

$$\boldsymbol{\eta}_{\mathbf{q},s}^T(\mathbf{r}) = (2\pi)^{-3/2} \hat{\mathbf{e}}_s(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}}, \quad s = 1, 2. \quad (14.62)$$

Here, the unit vectors $\hat{\mathbf{e}}_s(\mathbf{q})$ belonging to a given $\mathbf{q}$ are chosen as real and orthogonal, i.e., $\hat{\mathbf{e}}_s(\mathbf{q}) \cdot \hat{\mathbf{e}}_{s'}(\mathbf{q}) = \delta_{ss'}$. The plane waves in (14.62) form a continuous “orthonormal” basis. The orthonormality condition reads

$$(2\pi)^{-3} \int_{-\infty}^{\infty} \hat{\mathbf{e}}_s(\mathbf{q}) \cdot \hat{\mathbf{e}}_{s'}(\mathbf{q}') e^{i(\mathbf{q}-\mathbf{q}') \cdot \mathbf{r}} d^3 r = \delta_{ss'} \delta(\mathbf{q} - \mathbf{q}'), \quad (14.63)$$

and since

$$\sum_{s=1,2} \hat{\mathbf{e}}_s(\mathbf{q}) \hat{\mathbf{e}}_s(\mathbf{q}) = U - \hat{\mathbf{q}} \hat{\mathbf{q}}, \quad (14.64)$$

where $\hat{\mathbf{q}}$ is a unit vector in the $\mathbf{q}$ -direction, the completeness theorem takes the form

$$\delta_{\text{T}}(\mathbf{r} - \mathbf{r}_0) = (2\pi)^{-3} \int_{-\infty}^{\infty} (U - \hat{\mathbf{q}} \hat{\mathbf{q}}) e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)} d^3 q, \quad \mathbf{r} \neq \mathbf{r}_0. \quad (14.65)$$

The result in (14.65), which alternatively can be considered as a Fourier integral expansion of the transverse delta function, holds only for $\mathbf{r} \neq \mathbf{r}_0$, as indicated. A comparison of (14.49) and (14.61) immediately shows that the transverse propagator has the plane-wave expansion

$$\mathbf{G}_{\text{T}}(\mathbf{r} - \mathbf{r}_0; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \frac{U - \hat{\mathbf{q}} \hat{\mathbf{q}}}{q^2 - q_0^2} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)} d^3 q, \quad \mathbf{r} \neq \mathbf{r}_0. \quad (14.66)$$

Since

$$\delta(\mathbf{r} - \mathbf{r}_0) U = \frac{U}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)} d^3 q, \quad (14.67)$$

and $\delta_{\text{L}} = U\delta - \delta_{\text{T}}$, it appears that the longitudinal self-field propagator in (14.41) has the following plane-wave eigenvector expansion:

$$\mathbf{g}_{\text{L}}(\mathbf{r} - \mathbf{r}_0; \omega) = -(2\pi)^{-3} \int_{-\infty}^{\infty} \frac{\hat{\mathbf{q}} \hat{\mathbf{q}}}{q_0^2} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)} d^3 q, \quad \mathbf{r} \neq \mathbf{r}_0. \quad (14.68)$$

By insertion of (14.66) and (14.68) into (14.36) one obtains for the Green function $\mathbf{G}(\mathbf{R}; \omega)$ the eigenvector (Fourier integral) expansion

$$\mathbf{G}(\mathbf{r} - \mathbf{r}_0; \omega) = (2\pi)^{-3} \int_{-\infty}^{\infty} \left(\frac{U - \hat{\mathbf{q}} \hat{\mathbf{q}}}{q^2 - q_0^2} - \frac{\hat{\mathbf{q}} \hat{\mathbf{q}}}{q_0^2} \right) e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)} d^3 q, \quad \mathbf{r} \neq \mathbf{r}_0. \quad (14.69)$$

The Fourier transform of $\mathbf{G}(\mathbf{r} - \mathbf{r}_0; \omega)$ precisely is the one already determined by a somewhat different method in Sect. 4.2; see (4.28).

14.3 Contraction Geometry and Transverse Self-Field Dynamics

In Sect. 14.1.1, a transverse propagator description was established which in the spectral representation allows one to calculate a *part* of the transverse electric field from a microscopic current density distribution in space points *outside* the source

distribution; see (14.6). To understand why only a certain part of the transverse electric field is obtained via (14.6), I remind the reader of the analysis in Sect. 3.2.1. There, an integral expression for the *total* electric field valid outside the current density distribution was obtained (3.21). To determine the total field inside the source, the influence of the singularity of the integrand at $\mathbf{r} = \mathbf{r}'$ must be investigated with care. As we shall realize below, it turns out that the singular behavior of the integrand gives rise to an extra so-called self-field contribution to the total electric field. When this self-field is divided into its transverse and longitudinal vector-field parts, a transverse electric self-field appears not only inside the current density distribution but also in the entire rim zone.

14.3.1 Volume and Surface Integral Contributions to the Transverse Electric Field

Although it is possible first to determine the self-field contribution to the total electric field and then calculate the transverse self-field, it is instructive to determine the transverse self-field directly starting from the transverse set of Maxwell–Lorentz equations. The subsequent calculation of the transverse self-field is carried out in the space–frequency domain, and to lighten the notation the reference to the angular frequency will be omitted from the arguments of the various quantities.

The transverse electric field, $\mathbf{E}_T(\mathbf{r})$, satisfies the inhomogeneous Helmholtz equation in (13.1), and the transverse current density distribution, $\mathbf{J}_T(\mathbf{r})$, may be considered as the source of this field. By operating on this equation with $q_0^{-2}\nabla \times (\nabla \times)$, and interchanging the operators $q_0^{-2}\nabla \times (\nabla \times)$ and $\nabla^2 + q_0^2$ one obtains

$$(\nabla^2 + q_0^2) [q_0^{-2}\nabla \times (\nabla \times \mathbf{E}_T(\mathbf{r}))] = \frac{1}{i\epsilon_0\omega} \nabla \times (\nabla \times \mathbf{J}_T(\mathbf{r})). \quad (14.70)$$

Since $\nabla \times (\nabla \times \mathbf{E}_T) = -\nabla^2 \mathbf{E}_T$ it readily appears from (13.1) that (14.70) is equivalent to

$$(\nabla^2 + q_0^2) [\mathbf{E}_T(\mathbf{r}) - (i\epsilon_0\omega)^{-1} \mathbf{J}_T(\mathbf{r})] = (i\epsilon_0\omega)^{-1} \nabla \times (\nabla \times \mathbf{J}_T(\mathbf{r})). \quad (14.71)$$

In terms of the scalar propagator, $g(|\mathbf{r} - \mathbf{r}'|)$ the transverse field generated by the source thus is given by

$$\mathbf{E}_T(\mathbf{r}) = (i\epsilon_0\omega)^{-1} \left[\mathbf{J}_T(\mathbf{r}) - \lim_{\delta \rightarrow 0} \int_{V_\delta(\mathbf{r})}^{V_T} g(|\mathbf{r} - \mathbf{r}'|) \nabla' \times (\nabla' \times \mathbf{J}_T(\mathbf{r}')) d^3r' \right], \quad (14.72)$$

cf. the analysis carried out on the basis of Ewald–Oseen extinction theorem in Sects. 13.1 and 13.2. Before proceeding the mathematical calculation some remarks on the notation used and the result given in (14.72) are necessary. As it stands, the

integral extends over the entire volume V_T of the transverse current density distribution, yet with a (small) volume $V_\delta = V_\delta(\mathbf{r})$ surrounding the singularity of $g(|\mathbf{r} - \mathbf{r}'|)$ at $\mathbf{r}' = \mathbf{r}$ cut out. After the integration has been carried out $V_\delta(\mathbf{r})$ shrinks down around the point $\mathbf{r}$ while keeping its shape, “position” and orientation with respect to $\mathbf{r}$. If δ designates the maximum chord length of the exclusion volume its shrinkage to infinitesimal size is characterized by $\delta \rightarrow 0$. At this stage of our calculation the reference to an infinitesimal exclusion volume may seem superfluous due to the fact that the integral is absolutely convergent ($\mathbf{J}_T(\mathbf{r})$ is always nonsingular), as was already pointed out in the remarks below (13.22). However, because we want to “move” the double nabla operation from $\mathbf{J}_T(\mathbf{r}')$ to $g(|\mathbf{r} - \mathbf{r}'|)$ it proves crucial to retain the limiting process in explicit form, as we shall realize. We want to carry out some sort of double nabla operation on the Huygens propagator in order to introduce the transverse propagator in the general theory, and the thereby make contact to the partial result given in (14.6) for the transverse electric field. Since $\nabla' \times \mathbf{J}_T(\mathbf{r}') = \nabla' \times \mathbf{J}(\mathbf{r}')$ it appears that one under the integral sign may replace the transverse part of the current density with the total current density, $\mathbf{J}(\mathbf{r})$. In consequence, it is sufficient to integrate over the in general smaller volume V in which $\mathbf{J}(\mathbf{r}')$ is nonvanishing. For atoms, molecules and mesoscopic particles V is in general much smaller than V_T . In (14.72) appears a certain self-field contribution $\mathbf{J}_T(\mathbf{r})/(i\epsilon_0\omega)$ to $\mathbf{E}_T(\mathbf{r})$. This contribution, which is nonvanishing in the entire near-field zone, is in itself a transverse vector-field contribution. The integral contribution to $\mathbf{E}_T$ also is a transverse vector-field contribution. This must be so because it equals the difference between $\mathbf{J}_T(\mathbf{r})/(i\epsilon_0\omega)$ and $\mathbf{E}_T(\mathbf{r})$. The reader may also verify this by a direct calculation. In view of (14.1) it follows that

$$\mathbf{E}_T(\mathbf{r}) - (i\epsilon_0\omega)^{-1} \mathbf{J}_T(\mathbf{r}) = \mathbf{E}(\mathbf{r}) - (i\epsilon_0\omega)^{-1} \mathbf{J}(\mathbf{r}). \quad (14.73)$$

The inhomogeneous integral relation between $\mathbf{E}_T(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r})$ can therefore immediately be replaced by a form-identical relation between $\mathbf{E}(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$. This implies that several of the subsequent results relating $\mathbf{E}_T(\mathbf{r})$ to $\mathbf{J}_T(\mathbf{r})$ also holds as relations between $\mathbf{E}(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$.

Let us now temporarily introduce the abbreviation

$$\mathbf{F}(\mathbf{r}') \equiv \nabla' \times \mathbf{J}_T(\mathbf{r}'). \quad (14.74)$$

By utilizing the vector relation

$$g\nabla' \times \mathbf{F} = \nabla' \times (g\mathbf{F}) - (\nabla' g) \times \mathbf{F}, \quad (14.75)$$

and Gauss theorem in the form

$$\int_{\Omega} \nabla \times \mathbf{V} d\Omega = \int_S \hat{\mathbf{n}} \times \mathbf{V} dS, \quad (14.76)$$

where the vector $\mathbf{V}$ and its first derivatives are continuous over the simply connected domain Ω enclosed by the surface S , and $\hat{\mathbf{n}}$ denotes a unit normal vector on dS ,

directed outwards from Ω , the integral in (14.72) can be transformed as follows

$$\lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} g \nabla' \times \mathbf{F} d^3 r' = \lim_{\delta \rightarrow 0} \int_{S_\delta} \hat{\mathbf{n}}' \times (g \mathbf{F}) dS' - \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} (\nabla' g) \times \mathbf{F} d^3 r', \quad (14.77)$$

where $\hat{\mathbf{n}}' \equiv \hat{\mathbf{n}}(\mathbf{r}')$, and S_δ is the surface enclosing the exclusion volume V_δ . In applying Gauss theorem one also gets an integral over a surface enclosing V_T . This integral contribution vanishes because we choose a surface lying completely outside V_T . In the limit $\delta \rightarrow 0$ the integral over S_δ also vanishes since $g(|\mathbf{r} - \mathbf{r}'|)$ behaves as $|\mathbf{r} - \mathbf{r}'|^{-1}$ and the surface area element dS' as $|\mathbf{r} - \mathbf{r}'|^2$ for $\delta \rightarrow 0$. Hence, we have achieved the result

$$\lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} g \nabla' \times \mathbf{F} d^3 r' = - \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} (\nabla' g) \times \mathbf{F} d^3 r'. \quad (14.78)$$

The integrand on the right side of this equation can be rewritten in a form in which the Green function (propagator) for the magnetic field appears. To realize this one uses the identity

$$(\nabla' g) \times \mathbf{F} = [\nabla' \times (g \mathbf{U})] \cdot \mathbf{F} = -[\nabla \times (g \mathbf{U})] \cdot \mathbf{F}. \quad (14.79)$$

The above identity may be proven with the help of the Cartesian expansion of the unit dyadic, i.e.,

$$\mathbf{U} = \sum_i \hat{\mathbf{e}}_i \hat{\mathbf{e}}_i, \quad (14.80)$$

where $\hat{\mathbf{e}}_i$ is a unit vector along the i th Cartesian axis ($i = x, y, z$). Thus,

$$\begin{aligned} [\nabla' \times (g \mathbf{U})] \cdot \mathbf{F} &= \sum_i [\nabla' \times (g \hat{\mathbf{e}}_i)] \hat{\mathbf{e}}_i \cdot \mathbf{F} = \sum_i (\nabla' g \times \hat{\mathbf{e}}_i) \hat{\mathbf{e}}_i \cdot \mathbf{F} \\ &= (\nabla' g) \times \left(\sum_i \hat{\mathbf{e}}_i \hat{\mathbf{e}}_i \right) \cdot \mathbf{F} = (\nabla' g) \times \mathbf{F}. \end{aligned} \quad (14.81)$$

A comparison of (3.30) and (14.79) shows that

$$(\nabla' g) \times \mathbf{F} = -i q_0 \mathbf{G}_M \cdot \mathbf{F}. \quad (14.82)$$

Together, (14.72), (14.74), (14.78) and (14.82) give the following result for the transverse electric field:

$$\mathbf{E}_T(\mathbf{r}) = \frac{\mathbf{J}_T(\mathbf{r})}{i \epsilon_0 \omega} - \frac{1}{\epsilon_0 c_0} \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}_M(\mathbf{r} - \mathbf{r}') \cdot \nabla' \times \mathbf{J}_T(\mathbf{r}') d^3 r'. \quad (14.83)$$

By now we are left with the problem of “moving” the nabla operation from $\mathbf{J}_T$ to $\mathbf{G}_M$. To accomplish this goal it is easiest perhaps to make use of the dyadic

structure of $\mathbf{G}_M$, viz.,

$$\mathbf{G}_M = \sum_j \boldsymbol{\gamma}_j \hat{\mathbf{e}}_j = - \sum_j \hat{\mathbf{e}}_j \boldsymbol{\gamma}_j, \quad (14.84)$$

where

$$\boldsymbol{\gamma}_j = \sum_i \mathbf{G}_{M,ij} \mathbf{e}_i. \quad (14.85)$$

The second equality in (14.84) stems from the fact that $\mathbf{G}_M$ is antisymmetric. The reader may notice that an analogous expansion to the one above was made for the transverse Green function for a finite domain in relation to the establishment of the eigenfunction expansion for this Green function; see (14.51)–(14.53). A simple calculation gives

$$\begin{aligned} \nabla' \cdot (\mathbf{J}_T \times \mathbf{G}_M) &= \sum_j (\nabla') \cdot (\mathbf{J}_T \times \boldsymbol{\gamma}_j) \hat{\mathbf{e}}_j \\ &= \sum_j [(\nabla' \times \mathbf{J}_T) \cdot \boldsymbol{\gamma}_j \hat{\mathbf{e}}_j - \mathbf{J}_T \cdot (\nabla' \times \boldsymbol{\gamma}_j) \hat{\mathbf{e}}_j] \\ &= (\nabla' \times \mathbf{J}_T) \cdot \mathbf{G}_M - \mathbf{J}_T \cdot \nabla' \times \mathbf{G}_M \\ &= -\mathbf{G}_M \cdot (\nabla' \times \mathbf{J}_T) - (\nabla' \times \mathbf{G}_M) \cdot \mathbf{J}_T. \end{aligned} \quad (14.86)$$

The last step has made use of the fact that $\mathbf{G}_M$ and $\nabla' \times \mathbf{G}_M$ are antisymmetric and symmetric dyadics, respectively. The identity in (14.86) in combination with Gauss theorem (in its textbook form) show that the volume integral term in (14.83) can be transformed to

$$\begin{aligned} & - \lim_{\delta \rightarrow 0} \int_{V_\delta} \mathbf{G}_M \cdot \nabla' \times \mathbf{J}_T d^3 r' \\ &= \lim_{\delta \rightarrow 0} \left[\int^{S_\delta} \hat{\mathbf{n}}' \cdot (\mathbf{J}_T \times \mathbf{G}_M) dS' + \int_{V_\delta} (\nabla' \times \mathbf{G}_M) \cdot \mathbf{J}_T d^3 r' \right]. \end{aligned} \quad (14.87)$$

It is convenient for what follows to rewrite each of the two integrals on the right-hand side in (14.87). For the surface integral we use the identity

$$\hat{\mathbf{n}}' \cdot (\mathbf{J}_T \times \mathbf{G}_M) = -(\mathbf{G}_M \times \hat{\mathbf{n}}') \cdot \mathbf{J}_T \quad (14.88)$$

to obtain

$$\begin{aligned} \lim_{\delta \rightarrow 0} \int^{S_\delta} \hat{\mathbf{n}}' \cdot (\mathbf{J}_T \times \mathbf{G}_M) dS' &= - \lim_{\delta \rightarrow 0} \int^{S_\delta} (\mathbf{G}_M \times \hat{\mathbf{n}}') \cdot \mathbf{J}_T dS' \\ &= \left[- \lim_{\delta \rightarrow 0} \int^{S_\delta} \mathbf{G}_M \times \hat{\mathbf{n}}' dS' \right] \cdot \mathbf{J}_T(\mathbf{r}). \end{aligned} \quad (14.89)$$

The reader may easily prove (14.88) for herself with the help of (14.84). The second equality in (14.89) follows readily from the fact that $\mathbf{J}_T(\mathbf{r}')$ is nonsingular everywhere in space. The integrand of the volume integral can be rewritten in such a form that the standard Green function for the electric field, $\mathbf{G}$, appears instead of $\nabla' \times \mathbf{G}_M = -\nabla \times \mathbf{G}_M$. For this purpose we start from the expression given in (3.30) for $\mathbf{G}_M$. Thus,

$$\nabla' \times \mathbf{G}_M = \frac{i}{q_0} \nabla \times [\nabla \times (g\mathbf{U})]. \quad (14.90)$$

By means of the expansion in (14.84), and some straightforward vector manipulations one obtains

$$\begin{aligned} \nabla' \times \mathbf{G}_M &= \frac{i}{q_0} (\nabla \nabla g - U \nabla^2 g) \\ &= \frac{i}{q_0} (\nabla \nabla g + q_0^2 g \mathbf{U}). \end{aligned} \quad (14.91)$$

In taking the last step, the homogeneous Helmholtz equation satisfied for $g(|\mathbf{r} - \mathbf{r}'|)$ for $\mathbf{r} \neq \mathbf{r}'$, i.e., (13.2), was used. A comparison of (3.22) and (14.91) now leads to the conclusion that

$$\nabla' \times \mathbf{G}_M = i q_0 \mathbf{G}. \quad (14.92)$$

When the results in (14.89) and (14.92) are inserted into (14.87), we reach the following important equation for the transverse part of the microscopic electric field:

$$\begin{aligned} \mathbf{E}_T(\mathbf{r}) &= i \mu_0 \omega \lim_{\delta \rightarrow 0} \int_{V_\delta} \mathbf{G}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}_T(\mathbf{r}') d^3 r' \\ &\quad - \frac{1}{\epsilon_0 c_0} \left[\lim_{\delta \rightarrow 0} \int_{S_\delta} \mathbf{G}_M(\mathbf{r} - \mathbf{r}') \times \hat{\mathbf{n}}(\mathbf{r}') dS' \right] \cdot \mathbf{J}_T(\mathbf{r}) + \frac{\mathbf{J}_T(\mathbf{r})}{i \epsilon_0 \omega}. \end{aligned} \quad (14.93)$$

Let us now briefly discuss the central result in (14.93). The first term on the right-hand side of the equation relates $\mathbf{E}_T(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r}')$ in a spatially nonlocal manner. The kernel in this integral relation is the standard Green function. In the next subsection we shall see how the volume integral can be related to the integral for the transverse field outside the source region, i.e., (14.6). The second term in (14.92) represents a self-field contribution because it relates $\mathbf{E}_T(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r})$ in a spatially local fashion. The tensor in front of $\mathbf{J}_T(\mathbf{r})$ does not vanish in general, but the surface integral over S_δ depends on the geometry of the exclusion volume. In Sect. 14.3.3, we shall add the two self-field terms in (14.93), and thereby obtain a compact expression for the self-field dyadic relating $\mathbf{E}_T(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r})$ over the entire near-field domain. Since the surface integral over S_δ depends on the geometry of V_δ also the volume integral in (14.92) must depend on V_δ . This is so because the sum of the first two terms on the right side of (14.93) is independent of the exclusion volume, cf. the remarks made between (14.72) and (14.73).

14.3.2 The Connection Between the Volume Integral and the Exterior Solution for the Transverse Field

Since the point of observation ($\mathbf{r}$) in the volume integral in (14.93) always is located outside the domain of integration ($V_T - V_\delta$) one might perhaps expect that an exclusion-volume independent part of the same form as that given for exterior transverse field in (14.6) can be pulled out from the volume integral. In that case the remaining part of the volume integral must depend on the geometry of the exclusion volume. To demonstrate that this supposition in fact is correct let us insert the relation given in (14.7) between $\mathbf{G}(\mathbf{R}; \omega)$ and $\mathbf{G}_T(\mathbf{R}; \omega)$ into the volume integral. Thus, with ω reinserted in the various arguments for clarity,

$$\begin{aligned} & \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' \\ &= \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' \\ &+ q_0^{-2} \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \nabla \nabla g(|\mathbf{r} - \mathbf{r}'|; 0) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r'. \end{aligned} \quad (14.94)$$

Now, it turns out that the first integral on the right-hand side of (14.94) is independent of the geometry of the exclusion volume. To understand this it is sufficient to examine the form of the transverse propagator in the neighborhood of its singularity. Starting from the explicit form given in (14.9), insertion of the Taylor series expansion of the function $\exp(iq_0 R)$ around $q_0 R = 0$ leads after some algebraic calculations to the result

$$\mathbf{G}_T(\mathbf{R}; \omega) = (8\pi R)^{-1} (\mathbf{U} + \hat{\mathbf{R}} \hat{\mathbf{R}}) + \frac{iq_0}{6\pi} \mathbf{U} + \mathcal{O}(q_0 R). \quad (14.95)$$

The transverse propagator hence has a singularity of the R^{-1} -type. In consequence, the integral in question is absolutely convergent and thus independent of the geometry of the infinitesimal exclusion volume. The reference to the limiting process therefore can be neglected. Furthermore, we may extend the integral from V_T to the entire space since $\mathbf{J}_T(\mathbf{r}'; \omega)$ vanishes outside the rim zone. Altogether, we thus have

$$\lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' = \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r'. \quad (14.96)$$

Before proceeding with the transformation of (14.96) the following two remarks on the expression in (14.95) are appropriate: (1) The R -independent term $iq_0 \mathbf{U}/(6\pi)$ is identical to the one appearing in expansion of the standard Green function near $R = 0$; see (7.37). The radiation reaction field of an electric dipole (7.38) hence originates in the transverse propagator. (2) If the transverse propagator

is approximated by the first two terms in (14.95) its transversality is lost. Terms contained in $\mathcal{O}(q_0 R)$ are needed to restore the transversality.

At this stage, the folding theorem can be used on (14.96) to give

$$\int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{q}, \omega) \cdot \mathbf{J}_T(\mathbf{q}, \omega) e^{i\mathbf{q} \cdot \mathbf{r}} d^3 q, \quad (14.97)$$

and hereafter the expressions for $\mathbf{G}_T(\mathbf{q}; \omega)$ (see (14.66)) and $\mathbf{J}_T(\mathbf{q}; \omega)$ in terms of $\mathbf{J}(\mathbf{q}; \omega)$ (see (9.11)) lead to

$$\begin{aligned} \mathbf{G}_T(\mathbf{q}, \omega) \cdot \mathbf{J}_T(\mathbf{q}, \omega) &= \frac{U - \hat{\mathbf{q}}\hat{\mathbf{q}}}{q^2 - q_0^2} \cdot (U - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{J}(\mathbf{q}, \omega) \\ &= \mathbf{G}_T(\mathbf{q}, \omega) \cdot \mathbf{J}(\mathbf{q}, \omega). \end{aligned} \quad (14.98)$$

The folding theorem used once again finally results in

$$\int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' = \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r'. \quad (14.99)$$

By combining (14.8), (14.94), (14.96), and (14.99) it appears that the contribution to the transverse electric field from the volume integral in (14.93) can be divided as follows

$$\begin{aligned} & i\mu_0\omega \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r' \\ &= i\mu_0\omega \int_{-\infty}^{\infty} \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r' \\ &+ (i\epsilon_0\omega)^{-1} \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} (4\pi R^3)^{-1} (U - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3 r'. \end{aligned} \quad (14.100)$$

The first term on the right side of (14.100) precisely has the form obtained earlier (14.6) for the transverse field in points outside the source region (current density distribution $\mathbf{J}(\mathbf{r}'; \omega)$). The last volume integral in (14.100) carries the entire exclusion volume dependence.

14.3.3 Self-Field Dyadic

Let us now examine the last two terms on the right-hand side of (14.93). The sum of these terms constitutes the so-called (transverse) self-field, $\mathbf{E}_T^{\text{SF}}(\mathbf{r})$. The self-field at a given point ($\mathbf{r}$) in space only depends on the transverse current density at the same point, and it is convenient here to write the relation between $\mathbf{E}_T^{\text{SF}}(\mathbf{r})$ and $\mathbf{J}_T(\mathbf{r})$ in the form

$$\mathbf{E}_T^{\text{SF}}(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \mathbf{L} \cdot \mathbf{J}_T(\mathbf{r}; \omega), \quad (14.101)$$

where

$$\mathbf{L} = \mathbf{U} - iq_0 \lim_{\delta \rightarrow 0} \int^{S_\delta} \mathbf{G}_M(\mathbf{r} - \mathbf{r}'; \omega) \times \hat{\mathbf{n}}(\mathbf{r}') dS' \quad (14.102)$$

is the so-called self-field dyadic. To investigate the structure of $\mathbf{L}$ one inserts the expression given in (3.33) for the Green function for the magnetic field into (14.102). In the limit $\delta \rightarrow 0$, the term proportional to $(iq_0 R)^{-1}$ in $\mathbf{G}_M(\mathbf{R}; \omega)$ does not contribute to the surface integral (since dS' is proportional to R^2), and $\exp(iq_0 R) \rightarrow 1$. Thus, one obtains

$$\mathbf{L} = \frac{1}{4\pi} \lim_{\delta \rightarrow 0} \int^{S_\delta} (\mathbf{U} \times \hat{\mathbf{R}}) \times \hat{\mathbf{n}}(\mathbf{r}') \frac{dS'}{R^2} + \mathbf{U}. \quad (14.103)$$

With the help of the tensor relation

$$(\mathbf{U} \times \hat{\mathbf{R}}) \times \hat{\mathbf{n}}(\mathbf{r}') = \hat{\mathbf{n}}(\mathbf{r}') \hat{\mathbf{R}} - (\hat{\mathbf{n}}(\mathbf{r}') \cdot \hat{\mathbf{R}}) \mathbf{U}, \quad (14.104)$$

and the solid angle integration

$$\int^{S_\delta} \frac{\hat{\mathbf{n}}(\mathbf{r}') \cdot \hat{\mathbf{R}}}{R^2} dS' = 4\pi, \quad (14.105)$$

one realizes that

$$\mathbf{L} = \frac{1}{4\pi} \lim_{\delta \rightarrow 0} \int^{S_\delta} \frac{\hat{\mathbf{n}}(\mathbf{r}') \hat{\mathbf{R}}}{R^2} dS'. \quad (14.106)$$

The surface integral in (14.106) is independent of the size of the exclusion volume, it only depends on its form. Therefore, the limit procedure $\delta \rightarrow 0$ may be omitted from (14.106), and so we finally have

$$\mathbf{L} = \frac{1}{4\pi} \int^{S_\delta} \frac{\hat{\mathbf{n}}(\mathbf{r}') \hat{\mathbf{R}}}{R^2} dS'. \quad (14.107)$$

Let me remind the reader that $\hat{\mathbf{n}}(\mathbf{r}')$ at every point on S_δ is directed into the contraction volume V_δ , and that $\mathbf{R} = \mathbf{r} - \mathbf{r}'$.

It immediately appears from (14.107) that because the integrand is real the self-field dyadic $\mathbf{L}$ is real. The self-field dyadic also is symmetric, i.e.,

$$\int^{S_\delta} \left(\hat{\mathbf{n}}(\mathbf{r}') \hat{\mathbf{R}} - \hat{\mathbf{R}} \hat{\mathbf{n}}(\mathbf{r}') \right) \frac{dS'}{R^2} = \mathbf{0}. \quad (14.108)$$

The proof that (14.108) is correct can easily be given. For the arbitrary tensor element ij one thus has

$$\begin{aligned}
\int^{S_\delta} \left(\hat{\mathbf{n}}(\mathbf{r}') \hat{\mathbf{R}} - \hat{\mathbf{R}} \hat{\mathbf{n}}(\mathbf{r}') \right)_{ij} \frac{dS'}{R^2} &= \int^{S_\delta} \left(\hat{\mathbf{n}}(\mathbf{r}') \times \hat{\mathbf{R}} \right)_k \epsilon_{ijk} \frac{dS'}{R^2} \\
&= \int_{V_\delta}^{V_\infty} \left[\nabla' \times \left(\frac{\hat{\mathbf{R}}}{R^2} \right) \right]_k \epsilon_{ijk} dS' = 0. \quad (14.109)
\end{aligned}$$

The transformation from a surface to a volume integral was done using Gauss theorem in the form given in (14.76), and the last equality is a consequence of the fact that the curl of $\hat{\mathbf{R}}/R^2$ is zero. The symbol V_∞ denotes all space, and ϵ_{ijk} is element number (ijk) of the Levi–Civita tensor. Since $\mathbf{L}$ is a real symmetric dyadic a set of principal axes can be found. Referred to these $\mathbf{L}$ will be a diagonal dyadic. The trace of $\mathbf{L}$ is given by

$$\text{Tr}\{\mathbf{L}\} = \frac{1}{4\pi} \int^{S_\delta} \frac{\hat{\mathbf{n}}(\mathbf{r}') \cdot \hat{\mathbf{R}}}{R^2} dS', \quad (14.110)$$

and in the view of (14.105) it thus appears that

$$\text{Tr}\{\mathbf{L}\} = 1. \quad (14.111)$$

Referred to the principal axes the self-field dyadic hence can be written in terms of just two independent quantities.

14.4 Propagator Plus Self-Field Electrodynamics in the Rim Zone and Source Region

As a result of the analysis in Sect. 14.3 we have come to the conclusion that the transverse part of the microscopic electric field can be written in the form

$$\begin{aligned}
\mathbf{E}_T(\mathbf{r}; \omega) &= i\mu_0\omega \int^V \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r' \\
&+ (i\epsilon_0\omega)^{-1} \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \frac{1}{4\pi R^3} \left(\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}} \right) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3r' \\
&+ (i\epsilon_0\omega)^{-1} \mathbf{L} \cdot \mathbf{J}_T(\mathbf{r}; \omega), \quad (14.112)
\end{aligned}$$

as one immediately sees by combining (14.93) and (14.100)–(14.102). The first term on the right side of (14.112) is in itself divergence-free, whereas only the sum of the two last terms satisfies this criterion. Outside the transverse current density domain only the integral containing $\mathbf{G}_T(\mathbf{R}; \omega)$ survives, in agreement with the fact that the electromagnetic field is purely radiative here. The last two terms are both nonradiative, the first spatially nonlocal in its structure, and the second (self-field term) local (see Fig. 14.2). The balance between the two nonradiative contributions to $\mathbf{E}_T(\mathbf{r}; \omega)$ depends on the geometry of the contraction volume. The simplest systems of interest in near-field electrodynamics often have some kind of spatial symmetry.

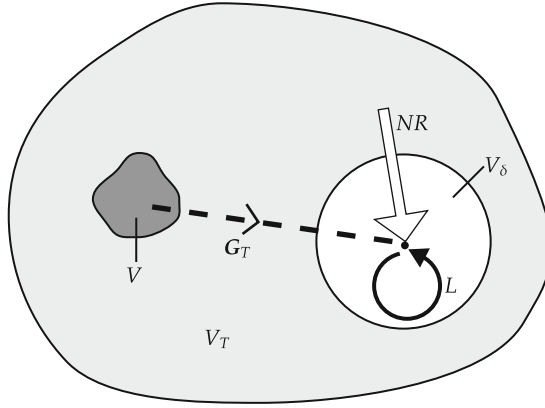


Fig. 14.2 Schematic illustration showing the radiative and nonradiative contributions to the transverse electric field at an observation point located in the rim zone (V_T) of a current density source (extension V): (1) A *radiative* contribution is described in terms of the transverse propagator $\mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega)$ [first term in (14.112)], (2) a spatially nonlocal *nonradiative* contribution (NR) comes from the rim zone outside the exclusion volume (V_δ) [second term in (14.112)], and (3) a local *self-field* contribution described in terms of the self-field dyadic, $\mathbf{L}$ (last term in (14.112)). Only the sum of the two nonradiative terms has a physical meaning, and the balance between them depends on the geometry of the contraction volume

For such systems a specific contraction geometry usually will be preferably to all others. More complicated systems in certain cases can be divided into subsystems each of which possesses their own spatial symmetry. Use of different contraction schemes for the individual subsystems may be advantageous then. In some situations, a choice between relevant contraction schemes has to be made. For what follows it is convenient to replace (14.112) by the expression

$$\begin{aligned} \mathbf{E}_T(\mathbf{r}; \omega) = & i\mu_0\omega \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_T(\mathbf{r}'; \omega) d^3r' \\ & + (i\epsilon_0\omega)^{-1} \mathbf{L} \cdot \mathbf{J}_T(\mathbf{r}; \omega). \end{aligned} \quad (14.113)$$

The equivalence of (14.112) and (14.113) follows from (14.100).

The starting point for the establishment of (14.113) was (14.72). In view of (14.73), and since $\nabla' \times \mathbf{J}_T(\mathbf{r}') = \nabla' \times \mathbf{J}(\mathbf{r}')$, the total electric field can be related to the current density as follows

$$\mathbf{E}(\mathbf{r}) = (i\epsilon_0\omega)^{-1} \left[\mathbf{J}(\mathbf{r}) - \lim_{\delta \rightarrow 0} \int_{V_\delta(\mathbf{r})}^V g(|\mathbf{r} - \mathbf{r}'|) \nabla' \times (\nabla' \times \mathbf{J}(\mathbf{r}')) d^3r' \right]. \quad (14.114)$$

The form-identity of (14.72) and (14.114), combined with the result in (14.113), immediately tell us that the total electric field in terms of the standard Green function, $\mathbf{G}(\mathbf{R}; \omega)$, and the self-field dyadic, $\mathbf{L}$, can be written in the form

$$\begin{aligned} \mathbf{E}(\mathbf{r}; \omega) = & i\mu_0\omega \lim_{\delta \rightarrow 0} \int_{V_\delta}^V \mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3r' \\ & + (i\epsilon_0\omega)^{-1} \mathbf{L} \cdot \mathbf{J}(\mathbf{r}; \omega). \end{aligned} \quad (14.115)$$

In a somewhat different (macroscopic) perspective the result in (14.115) was established three decades ago by Yaghjian [45]. If one subtracts (14.113) from (14.115) one obtains the following relation between the longitudinal parts of the electric field and current density:

$$\begin{aligned} \mathbf{E}_L(\mathbf{r}; \omega) = & i\mu_0\omega \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_L} \mathbf{G}(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}_L(\mathbf{r}'; \omega) d^3r' \\ & + (i\epsilon_0\omega)^{-1} \mathbf{L} \cdot \mathbf{J}_L(\mathbf{r}; \omega) \end{aligned} \quad (14.116)$$

Before the subtraction the integration domain in (14.115) is extended from V to V_T . This is possible because $\mathbf{J}(\mathbf{r}; \omega)$ is zero in the rim zone. Since the transverse and longitudinal current density domains are identical, one may of course, as is done in (14.116), replace V_T by V_L in the indication of the integration volume. A certain simplification occurs in (14.116) if one makes use of the relation between $\mathbf{G}$ and $\mathbf{G}_T$ ((14.7) with (14.8) inserted), and utilizes that

$$\lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_L} \mathbf{G}_T(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}_L(\mathbf{r}') d^3r' = \mathbf{0}. \quad (14.117)$$

The result in (14.117) must be correct because the relation between $\mathbf{E}_L(\mathbf{r})$ and $\mathbf{J}_L(\mathbf{r})$ is nonretarded. One may prove the result directly by inserting the plane-wave expansions for $\mathbf{G}_T(\mathbf{r} - \mathbf{r}')$, since $\mathbf{r} \neq \mathbf{r}'$ during the entire limiting process, $\delta \rightarrow 0$. We thus have

$$\begin{aligned} & \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_L} \mathbf{G}_T(\mathbf{r} - \mathbf{r}') \cdot \mathbf{J}_L(\mathbf{r}') d^3r' \\ &= (2\pi)^{-6} \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_L} \int_{-\infty}^{\infty} \frac{\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}}{q^2 - q_0^2} \cdot \hat{\mathbf{Q}}\hat{\mathbf{Q}} \cdot \mathbf{J}(\mathbf{Q}) e^{i\mathbf{q} \cdot \mathbf{r}} e^{i(\mathbf{Q}-\mathbf{q}) \cdot \mathbf{r}'} d^3Q d^3q d^3r'. \end{aligned} \quad (14.118)$$

The space integral may be extended from V_L to all space (V_∞) since $\mathbf{J}_L(\mathbf{r}')$ is zero outside V_L . After this extension, we change the order of integrations so as to carry out the $\mathbf{r}'$ -integration first. This integration gives

$$(2\pi)^{-3} \lim_{\delta \rightarrow 0} \int_{V_\delta(\mathbf{r})}^{V_\infty} e^{i(\mathbf{Q}-\mathbf{q}) \cdot \mathbf{r}'} d^3r' = (2\pi)^{-3} \int_{-\infty}^{\infty} e^{i(\mathbf{Q}-\mathbf{q}) \cdot \mathbf{r}'} d^3r' = \delta(\mathbf{Q} - \mathbf{q}), \quad (14.119)$$

because the integrand has no singularity at $\mathbf{r}' = \mathbf{r}$. The delta function $\delta(\mathbf{Q} - \mathbf{q})$ in turns allows one to perform the $\mathbf{Q}$ -integration. Hence, one ends up with an integral

$$(2\pi)^{-3} \int_{-\infty}^{\infty} (q^2 - q_0^2)^{-1} (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \hat{\mathbf{q}}\hat{\mathbf{q}} \cdot \mathbf{J}(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3q = \mathbf{0}, \quad (14.120)$$

which as indicated is zero due to the fact that $(\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \hat{\mathbf{q}}\hat{\mathbf{q}} = \mathbf{0}$. Altogether, the assertion in (14.117) has been proven. For the longitudinal field we therefore obtain the simplified result

$$\mathbf{E}_L(\mathbf{r}; \omega) = (i\epsilon_0\omega)^{-1} \left[\mathbf{L} \cdot \mathbf{J}_L(\mathbf{r}; \omega) + \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_L} \frac{\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}}{4\pi R^3} \cdot \mathbf{J}_L(\mathbf{r}'; \omega) d^3r' \right]. \quad (14.121)$$

As it stands, the nonretarded relation between $\mathbf{E}_L$ and $\mathbf{J}_L$ consists of a sum of spatially local and nonlocal parts. The division depends on the geometry of the contraction volume, but the sum is independent of the form of V_δ . We already know that the sum gives a spatially local relation between $\mathbf{E}_L$ and $\mathbf{J}_L$, namely the one in (14.1). The result in (14.121) is interesting however because of its close resemblance to the form of the nonretarded terms in the relation between $\mathbf{E}_T$ and $\mathbf{J}_T$; compare (14.112) and (14.121). From (14.1) and (14.121) follows the important identity

$$\mathbf{J}_L(\mathbf{r}) = \mathbf{L} \cdot \mathbf{J}_L(\mathbf{r}) + \lim_{\delta \rightarrow 0} \int_{V_\delta(\mathbf{r})}^{V_L} \frac{\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}}{4\pi R^3} \cdot \mathbf{J}_L(\mathbf{r}') d^3r', \quad (14.122)$$

with $\mathbf{L}$ given by the surface integral in (14.107).

14.5 Near-Field Electrodynamics in Spherical Contraction Geometry

Let us now determine the self-field dyadic in the case where the contraction volume is a sphere. The calculation is easily carried out in spherical coordinates (R, θ, ϕ) centered on $\mathbf{r}$. Thus, with

$$-\hat{\mathbf{n}}(\mathbf{r}') = -\hat{\mathbf{R}}(\mathbf{r}') = \hat{\mathbf{x}} \sin \theta \cos \phi + \hat{\mathbf{y}} \sin \theta \sin \phi + \hat{\mathbf{z}} \cos \theta, \quad (14.123)$$

and $dS' = R^2 \sin \theta d\theta d\phi$, inserted in (14.107) the integration over the azimuth angle ϕ immediately shows that

$$L_{xy} = L_{xz} = L_{yz} = 0. \quad (14.124)$$

Since the $\mathbf{L}$ -dyadic is symmetric only the tensor elements in the main diagonal are nonvanishing. The integrations over the polar angle θ are elementary, and we find

$$\mathbf{L} = \frac{1}{4} \int_0^\pi [(\hat{\mathbf{x}}\hat{\mathbf{x}} + \hat{\mathbf{y}}\hat{\mathbf{y}}) \sin^2 \theta + 2\hat{\mathbf{z}}\hat{\mathbf{z}} \cos^2 \theta] \sin \theta d\theta = \frac{\mathbf{U}}{3}. \quad (14.125)$$

The result in (14.125) could have been predicted without carrying out any explicit calculation. Thus, referred to Cartesian coordinates centered on $\mathbf{r}' = \mathbf{r}$ any orientation would constitute a set of principal axes for $\mathbf{L}$, and thus diagonalize the dyadic. For symmetry reasons the three diagonal elements of $\mathbf{L}$ must necessarily be equal, and equal to $1/3$, since the trace of $\mathbf{L}$ is unity.

The expression given in (14.112) for the transverse electric field becomes particularly simple in spherical contraction. Since $\mathbf{R} \neq \mathbf{0}$ in the second integral in (14.112), it appears from (9.20) that

$$\lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \frac{1}{4\pi R^3} (\mathbf{U} - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) \cdot \mathbf{J}_T(\mathbf{r}') d^3 r' = \lim_{\delta \rightarrow 0} \int_{V_\delta}^{V_T} \delta_L(\mathbf{R}) \cdot \mathbf{J}_T(\mathbf{r}') d^3 r' = \mathbf{0}. \quad (14.126)$$

The last equality follows from the fact that the longitudinal delta function picks out the longitudinal part of the subsequent vector function. In spherical contraction the transverse part of the microscopic electric field therefore is given by

$$\mathbf{E}_T(\mathbf{r}; \omega) = (3i\epsilon_0\omega)^{-1} \mathbf{J}_T(\mathbf{r}; \omega) + i\mu_0\omega \int^V \mathbf{G}_T(\mathbf{r} - \mathbf{r}'; \omega) \cdot \mathbf{J}(\mathbf{r}'; \omega) d^3 r'. \quad (14.127)$$

The result in (14.127) will be seen as part of a greater whole later on in this book.

14.6 Relativistic Covariance of the Huygens Propagator

The division of the electromagnetic field and the current density into their transverse and longitudinal vector-field parts is not relativistically invariant. The transverse electromagnetic propagator thus is not invariant under the Lorentz group of transformations. The standard Green functions for the electric- and magnetic field are not covariant tensors either. The Huygens propagator, however, *is* a covariant quantity as we shall realize below.

We begin by summarizing a few of the elements in the relativistic notation to be used in all later chapters. For the contravariant space-time four-vector with components x^μ ($\mu = 0, 1, 2, 3$) $x^0 = c_0 t$, $x^1 = x$, $x^2 = y$, $x^3 = z$, the notation

$$\{x^\mu\} = (c_0 t, \mathbf{r}) \quad (14.128)$$

is used. The associated covariant four-vector is written as

$$\{x_\mu\} = (c_0 t, -\mathbf{r}). \quad (14.129)$$

The relation between (14.128) and (14.129) corresponds to a metric tensor which elements are $g_{00} = -g_{11} = -g_{22} = -g_{33} = +1$. The definition of the metric tensor used here, and in the remaining part of the book, deviates with a factor of minus one from the definition used in Chap. 7. The fact that the speed of light is

the same in every inertial frame is expressed through the Lorentz invariance of the scalar product

$$(x, x) \equiv \sum_{\mu} x_{\mu} x^{\mu} = (c_0 t)^2 - x^2 - y^2 - z^2. \quad (14.130)$$

Often we shall assume that Greek indices which occur twice, once as subscript and once as superscript, are to be summed over from 0 to 3. Thus, we write e.g.,

$$(x, y) = x_{\mu} y^{\mu} = x^{\mu} y_{\mu} \quad (14.131)$$

for the relativistically invariant scalar product between the two sets $\{x^{\mu}\}$ and $\{y_{\mu}\}$ of space–time four-vectors.

Let us now consider the delta function $\delta[(x - x')^2]$, where, with $\tau = t - t'$ and $R = |\mathbf{r} - \mathbf{r}'|$,

$$(x - x')^2 \equiv (x_{\mu} - x'_{\mu})(x^{\mu} - x'^{\mu}) = c_0^2 \tau^2 - R^2. \quad (14.132)$$

By utilizing the relation $\delta(ax) = |a|^{-1} \delta(x)$ one obtains

$$\begin{aligned} \delta[(x - x')^2] &= \delta[(c_0 \tau - R)(c_0 \tau + R)] = \delta[2R(c_0 \tau - R)] + \delta[-2R(c_0 \tau + R)] \\ &= \frac{1}{2R} [\delta(c_0 \tau - R) + \delta(c_0 \tau + R)]. \end{aligned} \quad (14.133)$$

With the help of the Heaviside step function

$$\theta(x_0 - x'_0) = \theta[c_0(t - t')] = \frac{1}{c_0} \theta(\tau) \quad (14.134)$$

we can pick out the retarded ($\tau > 0$) part of (14.133). The quantity

$$D_R(x - x') \equiv \frac{1}{2\pi} \theta(x_0 - x'_0) \delta[(x - x')^2] \quad (14.135)$$

is the so-called covariant retarded (R) photon scalar propagator. It is clearly covariant since $\delta[(x - x')^2]$ is manifestly Lorentz invariant, and because the step function $\theta(x_0 - x'_0)$ is invariant against proper Lorentz transformations due to the fact that these cannot interchange past and future. By combining (14.133)–(14.135), it appears that $D_R(x - x')$ is related to the scalar propagator as follows:

$$g(R, \tau) [= \frac{1}{4\pi R} \delta\left(\frac{R}{c_0} - \tau\right)] = c_0 D_R(x - x'). \quad (14.136)$$

The relativistic covariance of the Huygens propagator hereby has been proven.

Chapter 15

Photon Wave Mechanics: Complex Field Theory

15.1 Wave Mechanics and the Einstein–de Broglie Relations

In quantum mechanics, free and in space completely unlocated particles all have wave functions of the generic form

$$[\psi](\mathbf{r}, t) = [\psi_0] \exp[i(\mathbf{q} \cdot \mathbf{r} - \omega t)] \quad (15.1)$$

in *configuration* space. The notation $[\psi]$ is meant to indicate that the wave function is a spinor. Thus, for a spinless particle the spinor has one component, for an electron described in the framework of the weakly relativistic Pauli theory it has two, and in the relativistic Dirac theory for a spin-1/2 particle the spinor has four components. For the photon, three, four, or six components exist depending on the framework used for the theory. Only if the “free” particle is confined to a finite region of space can the wavefunction be normalized. The spinoral amplitude $[\psi_0]$ is independent of $\mathbf{r}$ and t . Wave functions of the type in (15.1) are associated with particles of definite energy (E) and momentum ($\mathbf{p}$), namely

$$E = \hbar\omega, \quad (15.2)$$

and

$$\mathbf{p} = \hbar\mathbf{q}. \quad (15.3)$$

The Einstein–de Broglie relations in (15.2) and (15.3) express the particle-wave duality in quantum mechanics. Relativistic (special) mechanics leads to the following connection between the particle energy and momentum

$$E = \pm [(c_0 p)^2 + (mc_0^2)^2]^{1/2}, \quad (15.4)$$

where m is the particle’s rest mass, and $p = |\mathbf{p}|$. Particles have positive energy, and the plus sign must be used for these. Positive energy also means that $\omega > 0$, cf. (15.2). For antiparticles which all have negative energy, the minus sign in (15.4) has to be used, and $\omega < 0$. By inserting (15.2) and (15.3) into (15.4) one obtains the

two-branch dispersion relation

$$\omega = \pm c_0 [q^2 + Q_C^2]^{1/2}, \quad (15.5)$$

where

$$Q_C = \frac{mc_0}{\hbar} \quad (15.6)$$

is the Compton wave number of the particle (antiparticle), and $q = |\mathbf{q}|$. Moving with the speed of light the photon (antiphoton) eo ipso has zero rest mass. The fact that the forms of the photon and antiphoton dispersion relations

$$\omega = \pm c_0 q, \quad q > 0, \quad (15.7)$$

precisely are the same as the dispersion relations obtained from the free-space Maxwell equations suggests the possibility that the wave theory of Maxwell properly reformulated and interpreted may be considered as a wave mechanical theory of the photon (antiphoton). In this and the subsequent chapter, we shall in some detail examine to which extent this possibility exists. In a sense, it is clear from the outset that more is needed to establish a rigorous theory of the photon (antiphoton) because the free-space Maxwell equations do not contain Planck's constant. Before embarking on photon wave mechanics, let us see how the dispersion relations in (15.7) emerge from the free-space Maxwell equations

$$\nabla \times \mathbf{E}_T(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t), \quad (15.8)$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{r}, t), \quad (15.9)$$

$$\nabla \cdot \mathbf{E}_T(\mathbf{r}, t) = \nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0. \quad (15.10)$$

In free space, the electric field is, as we already know, a purely divergence-free vector field. I have emphasized this by the subscript T. It follows from (15.8)–(15.10) that the electric field satisfies the wave equation

$$\left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{E}_T(\mathbf{r}, t) = \mathbf{0}, \quad (15.11)$$

cf. (9.30). If the space–time Fourier integral

$$\mathbf{E}_T(\mathbf{r}, t) = (2\pi)^{-4} \int_{-\infty}^{\infty} \mathbf{E}_T(\mathbf{q}, \omega) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} d\omega d^3q, \quad (15.12)$$

is inserted into (15.11), the orthogonality of the various Fourier components shows that

$$\left[\left(\frac{\omega}{c_0} \right)^2 - q^2 \right] \mathbf{E}_T(\mathbf{q}, \omega) = \mathbf{0}. \quad (15.13)$$

Equation (15.13) immediately leads to the two-branch dispersion relation in (15.7).

15.2 Landau–Peierls Theory

The free-space dispersion relation for electromagnetic fields, allows one to make the decomposition

$$\mathbf{E}_T(\mathbf{q}, \omega) = 2\pi \left[\mathbf{E}_T^{(+)}(\mathbf{q}, c_0 q) \delta(\omega - c_0 q) + \mathbf{E}_T^{(-)}(\mathbf{q}, -c_0 q) \delta(\omega + c_0 q) \right]. \quad (15.14)$$

By inserting (15.14) into (15.12) one obtains

$$\mathbf{E}_T(\mathbf{r}, t) = \mathbf{E}_T^{(+)}(\mathbf{r}, t) + \mathbf{E}_T^{(-)}(\mathbf{r}, t), \quad (15.15)$$

where

$$\mathbf{E}_T^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{E}_T^{(+)}(\mathbf{q}, c_0 q) e^{i(\mathbf{q} \cdot \mathbf{r} - c_0 q t)} \frac{d^3 q}{(2\pi)^3}, \quad (15.16)$$

$$\mathbf{E}_T^{(-)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{E}_T^{(-)}(\mathbf{q}, -c_0 q) e^{i(\mathbf{q} \cdot \mathbf{r} + c_0 q t)} \frac{d^3 q}{(2\pi)^3}. \quad (15.17)$$

The complex field $\mathbf{E}_T^{(+)}(\mathbf{r}, t)$ represents the most general positive-frequency [superscript (+)] solution to the free-space Maxwell equations. Likewise, $\mathbf{E}_T^{(-)}(\mathbf{r}, t)$ is the general negative-frequency [superscript (–)] solution to these equations. Since the field $\mathbf{E}_T(\mathbf{r}, t)$ is real one must have

$$[\mathbf{E}_T^{(-)}(\mathbf{r}, t)]^* = \mathbf{E}_T^{(+)}(\mathbf{r}, t), \quad (15.18)$$

or equivalently

$$[\mathbf{E}_T^{(-)}(-\mathbf{q}, -c_0 q)]^* = \mathbf{E}_T^{(+)}(\mathbf{q}, c_0 q). \quad (15.19)$$

Due to (15.18), all information contained in the negative-frequency part of the spectrum thus is contained in the positive-frequency part, or to put it differently, antiphotons are identical to photons [229]. It is henceforth sufficient to consider only the $\mathbf{E}_T^{(+)}(\mathbf{r}, t)$ -signal. In the framework of statistical optics, a positive-frequency signal is called a complex analytical signal [53].

Originally, Landau and Peierls [214] considered $\mathbf{E}_T^{(+)}(\mathbf{r}, t)$ to be the quantum mechanical wave function of the photon in real space. Before we write down the wave equation satisfied by $\mathbf{E}_T^{(+)}(\mathbf{r}, t)$ it is convenient to introduce the nonlocal

operator $\sqrt{\Delta}$. This operator is defined by its action on a function

$$F(\mathbf{r}) = \int_{-\infty}^{\infty} F(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \frac{d^3q}{(2\pi)^3}. \quad (15.20)$$

Thus,

$$\sqrt{\Delta} F(\mathbf{r}) \equiv i \int_{-\infty}^{\infty} q F(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} \frac{d^3q}{(2\pi)^3}. \quad (15.21)$$

The symbolic notation $\sqrt{\Delta}$ is reasonable because repeated use of $\sqrt{\Delta}$ gives an operator identical to the Laplace operator, i.e.,

$$\sqrt{\Delta} \sqrt{\Delta} = \Delta \equiv \nabla^2, \quad (15.22)$$

as the reader may convince herself of by acting with $\sqrt{\Delta}$ on (15.21). By differentiating (15.16) with respect to time one obtains

$$\frac{\partial}{\partial t} \mathbf{E}_T^{(+)}(\mathbf{r}, t) = -c_0 \sqrt{\Delta} \mathbf{E}_T^{(+)}(\mathbf{r}, t). \quad (15.23)$$

Landau and Peierls considered (15.23) as the *unnormalized* wave equation of the photon in space–time. It may be shown that the positive-frequency part $\mathbf{B}^{(+)}(\mathbf{r}, t)$ of the magnetic field satisfies an equation form-identical to (15.23), namely,

$$\frac{\partial}{\partial t} \mathbf{B}^{(+)}(\mathbf{r}, t) = -c_0 \sqrt{\Delta} \mathbf{B}^{(+)}(\mathbf{r}, t). \quad (15.24)$$

Also $\mathbf{B}^{(+)}(\mathbf{r}, t)$ may therefore be taken as the photon wave function in space–time. In fact, various (complex) linear combinations of $\mathbf{E}^{(+)}(\mathbf{r}, t)$ and $\mathbf{B}^{(+)}(\mathbf{r}, t)$ may, and have, served as candidates for a photon wave function.

The connection between the Landau–Peierls equation for $\mathbf{E}_T^{(+)}(\mathbf{r}, t)$ and photon wave mechanics becomes distinct if (15.23) is transformed to the momentum (wave vector)–time representation. In view of (15.21), one immediately obtains

$$\frac{\partial}{\partial t} \mathbf{E}_T^{(+)}(\mathbf{q}; t) = -i c_0 q \mathbf{E}_T^{(+)}(\mathbf{q}; t), \quad (15.25)$$

and upon multiplication by $i\hbar$ then

$$i\hbar \frac{\partial}{\partial t} \mathbf{E}_T^{(+)}(\mathbf{q}; t) = c_0 \hbar q \mathbf{E}_T^{(+)}(\mathbf{q}; t). \quad (15.26)$$

It appears from (15.26) that the Landau–Peierls photon wave function $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ satisfies a wave equation of Hamiltonian (Schrödinger-like) form, the Hamilton operator being $\hat{H}(q) = c_0 p = c_0 \hbar q$. The time evolution of $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ is given by

$$\mathbf{E}_T^{(+)}(\mathbf{q}; t) = \mathbf{E}_T^{(+)}(\mathbf{q}; 0) \exp(-i c_0 q t), \quad (15.27)$$

and the stationary state evolution in (15.27) shows that a photon which is in an eigenstate for the momentum $\mathbf{p} = \hbar \mathbf{q}$ also is in an eigenstate for the energy. The energy is given by $E = c_0 p = c_0 \hbar q$, in accordance with the relativistic demand for a massless particle (see (15.4)). Since $\mathbf{q} \cdot \mathbf{E}_T^{(+)}(\mathbf{q}; t) = 0$, the vectorial photon wave function $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ always lies in a plane perpendicular to the direction of the photon momentum. The time development of the complex vector $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ characterizes the polarization state of the photon. In the space–time domain the three components of $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ are subjected to the constraint $\nabla \cdot \mathbf{E}_T^{(+)}(\mathbf{q}; t) = 0$, cf. (15.10). We shall discuss the photon polarization state later on in the framework of the so-called complex field theory.

The frequency independence of the speed of the light implies that a photon wave packet, formed by (weighed) superposition of plane-wave states in a small $\mathbf{q}$ -volume centered on a specific wave vector $\mathbf{q}$, propagates with a group velocity

$$\mathbf{v}_g = \nabla_{\mathbf{q}} \omega(\mathbf{q}) = c_0 \hat{\mathbf{q}}. \quad (15.28)$$

The photon wave packet thus moves in the $\mathbf{q}$ direction without dispersion, and with a speed equal to the vacuum speed of light, as one would have anticipated.

15.3 Interlude: Complex Analytical Signals

The Landau–Peierls theory presented in Sect. 15.2 has shown that the complex analytical signal concept plays an important role in photon wave mechanics. Before proceeding the quantum mechanical analysis of photon dynamics we briefly summarize the definition and a few of the basic properties of analytical signals. Let us assume that the real vector field $\mathbf{V}(\mathbf{r}, t)$ is square integrable in time, so that it at a given point in space can be represented as a Fourier integral

$$\mathbf{V}(\mathbf{r}, t) = (2\pi)^{-1} \int_{-\infty}^{\infty} \mathbf{V}(\mathbf{r}; \omega) e^{-i\omega t} d\omega. \quad (15.29)$$

The reality of $\mathbf{V}(\mathbf{r}, t)$ implies that the spectral amplitudes of positive and negative frequencies are related by

$$\mathbf{V}(\mathbf{r}; -\omega) = \mathbf{V}^*(\mathbf{r}; \omega). \quad (15.30)$$

The negative-frequency components of $\mathbf{V}(\mathbf{r}, t)$ thus do not carry any information not already contained in the positive-frequency components, or vice versa. The complex analytical signal, $\mathbf{V}^{(+)}(\mathbf{r}, t)$, is defined as the positive-frequency part of the Fourier integral in (15.29), i.e.,

$$\mathbf{V}^{(+)}(\mathbf{r}, t) = (2\pi)^{-1} \int_0^{\infty} \mathbf{V}(\mathbf{r}; \omega) e^{-i\omega t} d\omega. \quad (15.31)$$

With the definition

$$\mathbf{V}^{(+)}(\mathbf{r}; \omega) = \begin{cases} \mathbf{V}(\mathbf{r}; \omega) & , \quad \omega \geq 0 \\ \mathbf{0} & , \quad \omega < 0 \end{cases} , \quad (15.32)$$

Equation (15.31) can be written in the form

$$\mathbf{V}^{(+)}(\mathbf{r}, t) = (2\pi)^{-1} \int_{-\infty}^{\infty} \mathbf{V}^{(+)}(\mathbf{r}; \omega) e^{-i\omega t} d\omega. \quad (15.33)$$

The real ($\Re \mathbf{V}^{(+)}(\mathbf{r}, t)$) and imaginary ($\Im \mathbf{V}^{(+)}(\mathbf{r}, t)$) parts of the complex analytical signal form a Hilbert transform pair. To show this we start from the inverse transformation to (15.33), viz.,

$$\mathbf{V}^{(+)}(\mathbf{r}; \omega) = \int_{-\infty}^{\infty} \mathbf{V}^{(+)}(\mathbf{r}, t) e^{i\omega t} dt. \quad (15.34)$$

Thereafter, we compare this equation to the Fourier integral for the microscopic conductivity tensor, i.e.,

$$\sigma(t) = \int_{-\infty}^{\infty} \sigma(\omega) e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (15.35)$$

In Sect. 10.2.2, it was shown that causality, mathematically expressed by the condition $\sigma(t) = 0$ for $t < 0$, implies that $\sigma(\omega)$ is analytic in the *upper half* of the complex ω -plane. Since $\mathbf{V}^{(+)}(\mathbf{r}; \omega) = 0$ for $\omega < 0$, the *mathematical* analogy between (15.34) and (15.35) tells us that $\mathbf{V}^{(+)}(\mathbf{r}, t)$ must be analytic in the *lower half* of the complex t -plane. It is the sign difference between the exponents of the exponential functions in (15.34) and (15.35), which makes $\mathbf{V}^{(+)}(\mathbf{r}, t)$ analytic in the lower half plane instead of in the upper half plane. With the help of Cauchy's integral formula we were led to the result in (10.23). The corresponding result for the complex analytical signal hence must be the following:

$$P \int_{-\infty}^{\infty} \frac{\mathbf{V}^{(+)}(\mathbf{r}, t')}{t' - t} dt' = \pi i \mathbf{V}^{(+)}(\mathbf{r}, t), \quad (15.36)$$

remembering that the counter-clockwise contour integration now is along a contour located in the domain $\Im t \leq 0$ of the complex t -plane. In consequence of (15.36), it is obvious that $\Re \mathbf{V}^{(+)}(\mathbf{r}, t)$ and $\Im \mathbf{V}^{(+)}(\mathbf{r}, t)$ form a Hilbert transform pair, i.e.,

$$\Im \mathbf{V}^{(+)}(\mathbf{r}, t) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\Re \mathbf{V}^{(+)}(\mathbf{r}, t')}{t' - t} dt', \quad (15.37)$$

and

$$\Re \mathbf{V}^{(+)}(\mathbf{r}, t) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\Im \mathbf{V}^{(+)}(\mathbf{r}, t')}{t' - t} dt'. \quad (15.38)$$

For later purposes it is useful to seek to establish a direct relation between the real ($V(\mathbf{r}, t)$) and analytical ($V^{(+)}(\mathbf{r}, t)$) signals. To this end, one utilizes that

$$\Re V^{(+)}(\mathbf{r}, t) = \frac{1}{2} \left[V^{(+)}(\mathbf{r}, t) + \left(V^{(+)}(\mathbf{r}, t) \right)^* \right] = \frac{1}{2} V(\mathbf{r}, t). \quad (15.39)$$

The last equality in (15.39) appears as a consequence of (15.30), as the reader easily may convince himself of. By inserting (15.39) into (15.37) also the imaginary part of the analytical signal can be expressed in terms of $V(\mathbf{r}, t)$. Having obtained both $\Re V^{(+)}(\mathbf{r}, t)$ and $\Im V^{(+)}(\mathbf{r}, t)$ in terms of $V(\mathbf{r}, t)$ the following result emerges:

$$V^{(+)}(\mathbf{r}, t) = \frac{1}{2} \left[V(\mathbf{r}, t) + \frac{i}{\pi} P \int_{-\infty}^{\infty} \frac{V(\mathbf{r}, t')}{t' - t} dt' \right]. \quad (15.40)$$

The analytical signal thus is connected to the real signal by a relation which is nonlocal in time *but* local in space. Formally, one may write (15.40) in the compact form

$$V^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \delta^{(+)}(t - t') V(\mathbf{r}, t') dt', \quad (15.41)$$

where, with $t - t' = \tau$

$$\delta^{(+)}(\tau) = \frac{1}{2} \left(\delta(\tau) - \frac{i}{\pi} P \frac{1}{\tau} \right). \quad (15.42)$$

The integral relation between $V^{(+)}(\mathbf{r}, t)$ and $V(\mathbf{r}, t)$ can be expressed in a somewhat different form by inserting the inverse transformation to the one in (15.29) into (15.31). Hence, one obtains

$$V^{(+)}(\mathbf{r}, t) = \int_0^{\infty} \int_{-\infty}^{\infty} V(\mathbf{r}, t') e^{i\omega(t'-t)} dt' \frac{d\omega}{2\pi}. \quad (15.43)$$

Upon interchange of the t' and ω -integrations, a comparison to (15.41) shows that

$$\delta^{(+)}(\tau) = (2\pi)^{-1} \int_0^{\infty} e^{-i\omega\tau} d\omega. \quad (15.44)$$

The singular function $\delta^{(+)}(\tau)$ thus is just the positive-frequency part of the Dirac delta function, here represented by a superposition

$$\delta(\tau) = (2\pi)^{-1} \int_{-\infty}^{\infty} e^{-i\omega\tau} d\omega, \quad (15.45)$$

which has a minus sign in the argument of the exponential function.

15.4 Complex Field Theory in the Momentum–Time Domain

The Landau–Peierls photon wave function certainly not is the only possible candidate for a photon wave function. Other choices can be made which satisfy the free space Maxwell equations, and carry all information contained in these equations. In the present section, a particularly interesting choice which accentuates the photon helicity concept is studied. The photon wave mechanical formalism described below in the momentum–time representation, and in Sect. 15.5 in the space–time domain, is called the complex field theory of the photon, or just the CF theory. In relation to the CF theory also the normalization of the photon wave function will be addressed.

15.4.1 Photon Helicity Unit Vectors

Before embarking on the CF theory let us briefly discuss the polarization states of plane waves satisfying the free-space Maxwell equations. In reciprocal space, these equations are

$$\frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{q}; t) = i c_0^2 \mathbf{q} \times \mathbf{B}(\mathbf{q}; t), \quad (15.46)$$

$$\frac{\partial}{\partial t} \mathbf{B}(\mathbf{q}; t) = -i \mathbf{q} \times \mathbf{E}_T(\mathbf{q}; t), \quad (15.47)$$

with the transversality conditions

$$\mathbf{q} \cdot \mathbf{E}_T(\mathbf{q}; t) = \mathbf{q} \cdot \mathbf{B}(\mathbf{q}; t) = 0, \quad (15.48)$$

cf. (9.34) and (9.35). Since the complex field vectors $\mathbf{E}_T(\mathbf{q}; t)$ and $\mathbf{B}(\mathbf{q}; t)$ are both perpendicular to the wave vector $\mathbf{q}$, they can be expanded after two orthogonal unit (basis) vectors located in a plane normal to $\hat{\mathbf{q}}$. We assume tentatively that these unit vectors, denoted by $\hat{\epsilon}_1^R$ and $\hat{\epsilon}_2^R$, are real (superscript R), and that $\hat{\mathbf{q}}$, $\hat{\epsilon}_1^R$, and $\hat{\epsilon}_2^R$ in this order form a right-handed set. The transversality, orthonormality and right-handedness are expressed by the conditions

$$\hat{\mathbf{q}} \cdot \hat{\epsilon}_s^R = 0, \quad s = 1, 2 \quad (15.49)$$

$$\hat{\epsilon}_s^R \cdot \hat{\epsilon}_{s'}^R = \delta_{ss'}, \quad s, s' = 1, 2 \quad (15.50)$$

$$\hat{\epsilon}_1^R \times \hat{\epsilon}_2^R = \hat{\mathbf{q}}. \quad (15.51)$$

The completeness of the basis vectors in 2D is expressed through the dyadic expansion

$$\sum_{s=1,2} \hat{\epsilon}_s^R \hat{\epsilon}_s^R = \mathbf{U} - \hat{\mathbf{q}} \hat{\mathbf{q}}. \quad (15.52)$$

Let us now introduce a particular set of new complex basis vectors, $\hat{\mathbf{e}}_+$ and $\hat{\mathbf{e}}_-$, by means of the transformation

$$\hat{e}_+ = \frac{1}{\sqrt{2}}(\hat{e}_1^R + i\hat{e}_2^R), \quad (15.53)$$

$$\hat{e}_- = \frac{1}{\sqrt{2}}e^{i\delta}(i\hat{e}_1^R + \hat{e}_2^R). \quad (15.54)$$

The transformation is a so-called one-parameter transformation since it contains one free parameter, viz. the real phase parameter δ . The vectors $\hat{e}_+$ and $\hat{e}_-$ are complex unit vectors because

$$\hat{e}_+ \cdot \hat{e}_+^* = \hat{e}_- \cdot \hat{e}_-^* = 1, \quad (15.55)$$

and they are mutually orthogonal since

$$\hat{e}_+ \cdot \hat{e}_-^* (= \hat{e}_+^* \cdot \hat{e}_-) = 0. \quad (15.56)$$

The 2D-completeness follows from the dyadic relation

$$\hat{e}_+ \hat{e}_+^* + \hat{e}_- \hat{e}_-^* = \mathbf{U} - \hat{q} \hat{q}. \quad (15.57)$$

To prove (15.57) one inserts (15.53) and (15.54) into the left-hand side of (15.57), and makes use of (15.52) thereafter. The unit vector $\hat{e}_+$ describes a right-hand circularly polarized time-harmonic wave (clockwise rotation seen in the direction of $\hat{q}$), as it is well known. Independent of δ , $\hat{e}_-$ describes a left-hand circular polarization state. In relation to photon wave mechanics $\hat{e}_+$ and $\hat{e}_-$ are called helicity unit vectors since they relate to plane-wave photon states which are eigenstates for the photon helicity operator, the eigenvalue being $+1$ or -1 , respectively. To understand the physical role of the phase parameter δ in (15.54) let us compare the instantaneous orientations of the polarization unit vectors which in complex notation are given by $\hat{e}_+$ and $\hat{e}_-$. At a given time t the two real polarization vectors are

$$\Delta_{\pm}(t) = \Re \{ \hat{e}_{\pm} e^{-i\omega t} \}, \quad (15.58)$$

and by insertion of the expressions in (15.53) and (15.54) one obtains

$$\Delta_+(t) = \frac{1}{\sqrt{2}} \left[\hat{e}_1^R \cos \omega t + \hat{e}_2^R \sin \omega t \right], \quad (15.59)$$

$$\Delta_-(t) = \frac{1}{\sqrt{2}} \left[\hat{e}_1^R \sin(\omega t - \delta) + \hat{e}_2^R \cos(\omega t - \delta) \right]. \quad (15.60)$$

Since the two unit vectors rotate in opposite directions with the same constant angular velocity, ω , they will point in the same direction twice in a full revolution. A simple calculation shows that the polarization vectors overlap at angles which measured (counter-clockwise) from the $\hat{e}_1^R$ -direction are

$$\phi_1 = \frac{\pi}{4} + \frac{\delta}{2}, \quad (15.61)$$

and $\phi_2 = \phi_1 + \pi$. The phase parameter δ hence characterizes the overlap directions. When δ varies from 0 to 2π , ϕ_1 goes from $\pi/4$ to $3\pi/4$.

15.4.2 Photon Helicity Eigenstates: Wave Function and Wave Equations

We know from the analyses in Sects. 15.1 and 15.2 that the free-space Maxwell equations in reciprocal space are satisfied by the following positive-frequency ($\omega = +c_0q > 0$) solutions for the electric and magnetic fields:

$$\mathbf{E}_T^{(+)}(\mathbf{q}; t) = \mathbf{E}_T^{(+)}(\mathbf{q}, c_0q) e^{-ic_0qt}, \quad (15.62)$$

$$\mathbf{B}^{(+)}(\mathbf{q}; t) = \mathbf{B}^{(+)}(\mathbf{q}, c_0q) e^{-ic_0qt}, \quad (15.63)$$

with

$$\mathbf{B}^{(+)}(\mathbf{q}, c_0q) = c_0^{-1} \hat{\mathbf{q}} \times \mathbf{E}_T^{(+)}(\mathbf{q}, c_0q). \quad (15.64)$$

To within an arbitrary complex constant, (15.62)–(15.64) represent the general solution for the electromagnetic field for $\omega > 0$. In relation to photon wave mechanics, the constant must have a specific magnitude in order for the photon wave function to be normalized, as we shall realize later on. To remind ourselves that we in case are dealing with a normalized wave function small letters will be used below for the associated positive-frequency electric and magnetic field vectors that is $\mathbf{e}_T^{(+)}(\mathbf{q}; t)$ and $\mathbf{b}^{(+)}(\mathbf{q}; t)$.

In the CF theory discussed now, the photon helicity concept is accentuated. We begin by defining two so-called complex field vectors, $\boldsymbol{\beta}_+^{(+)}(\mathbf{q}; t)$ and $\boldsymbol{\beta}_-^{(+)}(\mathbf{q}; t)$ as follows:

$$\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t) = \frac{(2\pi)^{-3/2}}{N_{\beta}(q)} \left(\mathbf{e}_T^{(+)}(\mathbf{q}; t) \pm ic_0 \mathbf{b}^{(+)}(\mathbf{q}; t) \right), \quad (15.65)$$

where

$$N_{\beta}(q) = 2 \left(\frac{\hbar c_0 q}{\epsilon_0} \right)^{1/2} \quad (15.66)$$

is a q -dependent normalization coefficient. As we shall see in Sect. 15.4.4, the value of this coefficient has been chosen in such a manner that the mean values of the photon energy and momentum take familiar quantum mechanical forms. To derive dynamical evolution equations for the complex field vectors one uses the fact that the analytical vector fields $\mathbf{E}_T^{(+)}(\mathbf{q}; t)$ and $\mathbf{B}^{(+)}(\mathbf{q}; t)$ satisfy dynamical equations of the same form as the free space Maxwell equations that is

$$\frac{\partial}{\partial t} \mathbf{E}_T^{(+)}(\mathbf{q}; t) = ic_0^2 \mathbf{q} \times \mathbf{B}^{(+)}(\mathbf{q}; t), \quad (15.67)$$

$$\frac{\partial}{\partial t} \mathbf{B}^{(+)}(\mathbf{q}; t) = -i \mathbf{q} \times \mathbf{E}_T^{(+)}(\mathbf{q}; t), \quad (15.68)$$

and in addition the transversality conditions

$$\mathbf{q} \cdot \mathbf{E}_T^{(+)}(\mathbf{q}; t) = \mathbf{q} \cdot \mathbf{B}^{(+)}(\mathbf{q}; t) = 0. \quad (15.69)$$

The reader may easily prove (15.67) and (15.68) by means of (15.62)–(15.64). The single-photon field vectors $\mathbf{e}_T^{(+)}(\mathbf{q}; t)$ and $\mathbf{b}^{(+)}(\mathbf{q}; t)$ of course also satisfy dynamical equations of the forms given in (15.67) and (15.68), and a combination of the differential equations for these field vectors leads after some simple algebra to the following dynamical equations for the complex field vectors:

$$i\hbar \frac{\partial}{\partial t} \beta_{\pm}^{(+)}(\mathbf{q}; t) = \pm i c_0 \hbar q \hat{\mathbf{q}} \times \beta_{\pm}^{(+)}(\mathbf{q}; t). \quad (15.70)$$

If one make the ansatz's

$$\beta_{\pm}^{(+)}(\mathbf{q}; t) = \beta_{\pm}^{(+)}(\mathbf{q}; t) \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) \quad (15.71)$$

in the equations in (15.70), and utilizes that the helicity unit vectors satisfy the relations

$$\hat{\mathbf{q}} \times \hat{\mathbf{e}}_{\pm} = \mp i \hat{\mathbf{e}}_{\pm}, \quad (15.72)$$

[easily obtained via (15.51), (15.53), and (15.54)], it appears that the scalar amplitudes $\beta_{\pm}^{(+)}$ obey the same Schrödinger-like equation, viz.,

$$i\hbar \frac{\partial}{\partial t} \beta_{\pm}^{(+)}(\mathbf{q}; t) = c_0 \hbar q \beta_{\pm}^{(+)}(\mathbf{q}; t). \quad (15.73)$$

In the complex field theory, $\beta_{+}^{(+)}(\mathbf{q}; t)$ and $\beta_{-}^{(+)}(\mathbf{q}; t)$ are considered to be quantum mechanical wave functions for photons of positive and negative helicity, respectively. In the momentum (wave-vector) representation where the photon momentum operator $\hat{\mathbf{p}} = \hbar \hat{\mathbf{q}}$ is mathematically identical to the momentum itself, i.e., $\hat{\mathbf{p}} = \mathbf{p}$ ($\hat{\mathbf{q}} = \mathbf{q}$ also), the photon Hamilton operator on the right-hand side of (15.73) has the expected form $\hat{H} = c_0 \hbar q = c_0 p$. It also appears from (15.73) that the two helicity eigenstates have the same energy.

15.4.3 Photon Spinor Description

Seen in the perspective of relativistic quantum mechanics, one-photon states are, in the momentum representation, adequately classified according to their transformation under the inhomogeneous Lorentz group. The components of the energy–momentum four-vector all commute with each other, and it is therefore natural to characterize the photon state vectors in terms of the eigenvectors for the four-momentum operator. The internal state of the photon we characterize by means of

the helicity. Since the helicity of a massless particle, here a photon, is a Lorentz-invariant, the internal state of a photon of a given helicity looks the same in all inertial frames. Other one-photon states can be formed by linear superposition of the one-photon states with opposite helicities. It can be shown that a state formed by such a superposition in general will be changed by a Lorentz transformation into a different superposition. In free space, the two helicity wave functions, $\beta_{\pm}^{(+)}(\mathbf{q}; t)$, develop dynamically independent of each other. Photon wave mechanics is useful also for the understanding of photon-matter interactions, as we shall realize later on. When a photon for instance is scattered elastically from, say, an atom or a mesoscopic object, the two helicity states will in general couple during the interaction process. Viewed in the aforementioned perspective it is fruitful to consider the two vectorial helicity wave functions $\beta_{\pm}^{(+)}(\mathbf{q}; t)$ (15.71) as the upper and lower (vectorial) component of a generalized spinorial photon wave function. The spinor description of photon wave mechanics henceforth is formulated in analogy to the well known spinor description of massive spin-1/2 particles, e.g., electrons.

In the complex field (CF) theory, we consider the six-component object

$$[\Phi^{\text{CF}}](\mathbf{p}; t) \equiv \Phi^{\text{CF}}(\mathbf{p}; t) = \frac{1}{\hbar^{3/2}} \begin{pmatrix} \beta_{+}^{(+)}(\mathbf{p}/\hbar; t) \hat{e}_{+}(\hat{\mathbf{p}}) \\ \beta_{-}^{(+)}(\mathbf{p}/\hbar; t) \hat{e}_{-}(\hat{\mathbf{p}}) \end{pmatrix} \quad (15.74)$$

to be the photon wave function in the momentum representation. In emphasizing the $\mathbf{p}$ -representation instead of the equivalent $\mathbf{q}$ -representation, certain factors containing $\hbar$ appears, cf., the $\mathbf{p} = \hbar\mathbf{q}$ relation. If $(\Phi^{\text{CF}}(\mathbf{p}; t))^{\dagger}$ denotes the complex conjugate (row) vector to $\Phi^{\text{CF}}(\mathbf{p}; t)$ the photon wave function is normalized provided

$$\int_{-\infty}^{\infty} (\Phi^{\text{CF}}(\mathbf{p}; t))^{\dagger} \cdot \Phi^{\text{CF}}(\mathbf{p}; t) d^3 p = 1. \quad (15.75)$$

Because the helicity unit vectors satisfy (15.55), the normalization condition can also be expressed in the form

$$\int_{-\infty}^{\infty} [|\beta_{+}^{(+)}(\mathbf{q}; t)|^2 + |\beta_{-}^{(+)}(\mathbf{q}; t)|^2] d^3 q = 1. \quad (15.76)$$

Since

$$\beta_{\pm}^{(+)} = \beta_{\pm}^{(+)} \cdot (U - \hat{\mathbf{q}}\hat{\mathbf{q}}) = \beta_{\pm}^{(+)} \cdot (\hat{\mathbf{e}}_{+}^{*}\hat{\mathbf{e}}_{+} + \hat{\mathbf{e}}_{-}^{*}\hat{\mathbf{e}}_{-}), \quad (15.77)$$

where the first equality follows from the transversality of the $\beta_{\pm}^{(+)}$'s, and the second from (15.57), it follows that the scalar amplitudes (15.71) are given by

$$\beta_{\pm}^{(+)}(\mathbf{q}; t) = \beta_{\pm}^{(+)}(\mathbf{q}; t) \cdot \hat{\mathbf{e}}_{\pm}^{*}(\hat{\mathbf{q}}). \quad (15.78)$$

By combining (15.65), (15.66), (15.74), and (15.78) it is seen that the spinorial photon wave function in terms of the single-photon field vectors is given by

$$\Phi^{\text{CF}}(\mathbf{p}; t) = \frac{1}{2} \epsilon_0^{1/2} \hbar^{-3/2} (c_0 p)^{-1/2} \begin{pmatrix} \left[\mathbf{e}_T^{(+)}(\mathbf{p}/\hbar; t) + i c_0 \mathbf{b}^{(+)}(\mathbf{p}/\hbar; t) \right] \cdot \hat{\mathbf{e}}_+^*(\hat{\mathbf{p}}) \hat{\mathbf{e}}_+(\hat{\mathbf{p}}) \\ \left[\mathbf{e}_T^{(+)}(\mathbf{p}/\hbar; t) - i c_0 \mathbf{b}^{(+)}(\mathbf{p}/\hbar; t) \right] \cdot \hat{\mathbf{e}}_-^*(\hat{\mathbf{p}}) \hat{\mathbf{e}}_-(\hat{\mathbf{p}}) \end{pmatrix} \quad (15.79)$$

The free-space Maxwell equations in (15.67) and (15.68) determine the analytical field vectors to within an overall complex constant $C = |C| \exp(i\alpha)$. In retrospect it thus appears that the magnitude $|C|$ of this constant is determined in such a manner that the normalization condition in (15.75) is fulfilled. The solution to (15.67) and (15.68) that satisfies this condition was denoted by $(\mathbf{e}_T^{(+)}, \mathbf{b}^{(+)})$. Different choices of the phase factor $\exp(i\alpha)$ just result in different overall phase factors of modulus one on Φ^{CF} . These phase factors are of no physical importance.

By introduction of the supermatrix Hamiltonian

$$\mathcal{H}(\mathbf{p}) \equiv \begin{pmatrix} U - \hat{\mathbf{p}}\hat{\mathbf{p}} & \mathbf{0} \\ \mathbf{0} & U - \hat{\mathbf{p}}\hat{\mathbf{p}} \end{pmatrix} c_0 p, \quad (15.80)$$

a 6×6 matrix, the reader may with the help of (15.71), (15.73), and (15.74) verify that the spinorial CF photon wave function satisfies the Schrödinger-like wave equation

$$i\hbar \frac{\partial}{\partial t} \Phi^{\text{CF}}(\mathbf{p}; t) = \mathcal{H}(\mathbf{p}) \cdot \Phi^{\text{CF}}(\mathbf{p}; t) \quad (15.81)$$

in the momentum representation.

15.4.4 Quantum Mechanical Mean Values of the Photon Energy and Momentum

The general expression for the energy of the transverse part of the electromagnetic field, H_{trans} was given in (9.70). To obtain the energy in the one-photon field, in the following denoted by E , one just needs to replace $(\mathbf{E}_T, \mathbf{B})$ by $(\mathbf{e}_T^{(+)}, \mathbf{b}^{(+)})$ in (9.70). By utilizing the Parseval–Plancherel identity (9.56) the one-photon energy can be expressed as an integral over $\mathbf{q}$ -space, viz.,

$$E = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[\left(\mathbf{e}_T^{(+)}(\mathbf{q}; t) \right)^* \cdot \mathbf{e}_T^{(+)}(\mathbf{q}; t) + c_0^2 \left(\mathbf{b}^{(+)}(\mathbf{q}; t) \right)^* \cdot \mathbf{b}^{(+)}(\mathbf{q}; t) \right] \frac{d^3 q}{(2\pi)^3}. \quad (15.82)$$

From the equations in (15.65) one gets

$$\mathbf{e}_T^{(+)}(\mathbf{q}; t) = (2\pi)^{3/2} \frac{N_{\beta}(\mathbf{q})}{2} \left(\boldsymbol{\beta}_+^{(+)}(\mathbf{q}; t) + \boldsymbol{\beta}_-^{(+)}(\mathbf{q}; t) \right), \quad (15.83)$$

$$\mathbf{b}^{(+)}(\mathbf{q}; t) = (2\pi)^{3/2} \frac{N_{\beta}(q)}{2ic_0} \left(\boldsymbol{\beta}_+^{(+)}(\mathbf{q}; t) - \boldsymbol{\beta}_-^{(+)}(\mathbf{q}; t) \right), \quad (15.84)$$

and by inserting these relation into (15.82) we obtain

$$E = \frac{\epsilon_0}{4} \int_{-\infty}^{\infty} N_{\beta}^2(q) \left[\left(\boldsymbol{\beta}_+^{(+)} \right)^* \cdot \boldsymbol{\beta}_+^{(+)} + \left(\boldsymbol{\beta}_-^{(+)} \right)^* \cdot \boldsymbol{\beta}_-^{(+)} \right] d^3q. \quad (15.85)$$

By means of (15.55) and (15.71) one finds

$$\left(\boldsymbol{\beta}_{\pm}^{(+)} \right)^* \cdot \boldsymbol{\beta}_{\pm}^{(+)} = |\boldsymbol{\beta}_{\pm}^{(+)}|^2, \quad (15.86)$$

and the energy hence can be given in terms of the scalar amplitudes of the two helicity states. By inserting also the explicit expression for $N_{\beta}(q)$ (15.66) the one-photon energy finally takes the beautiful form

$$E = \int_{-\infty}^{\infty} \hbar c_0 q \left[\sum_{s=+,-} \left(\beta_s^{(+)}(\mathbf{q}; t) \right)^* \beta_s^{(+)}(\mathbf{q}; t) \right] d^3q. \quad (15.87)$$

The photon energy thus appears as the sum of the quantum mechanical mean values of the energy operator $\hbar c_0 q$ for the two helicity states. The one-photon normalization condition is given in (15.76). The result in (15.87) thus justifies the choice made for the normalization coefficient $N_{\beta}(q)$ in (15.66).

The momentum $\mathbf{P}_{\text{trans}}$ associated with the transverse electromagnetic field was given in (9.81). For the one-photon state the associated momentum is denoted by $\mathbf{P}$, and it is given by the following integral over $\mathbf{q}$ -space:

$$\mathbf{P} = \epsilon_0 \int_{-\infty}^{\infty} \left(\mathbf{e}_T^{(+)}(\mathbf{q}; t) \right)^* \times \mathbf{b}^{(+)}(\mathbf{q}; t) \frac{d^3q}{(2\pi)^3}. \quad (15.88)$$

The complex field vectors now are introduced in (15.88) by means of (15.83) and (15.84). Since

$$\hat{\mathbf{e}}_+^* \times \hat{\mathbf{e}}_- = \hat{\mathbf{e}}_+ \times \hat{\mathbf{e}}_-^* = \mathbf{0}, \quad (15.89)$$

as the reader readily may prove from (15.53) and (15.54), the two helicity eigenstates do not couple in the expression for $\mathbf{P}$, and one hence has

$$\mathbf{P} = \frac{\epsilon_0}{4ic_0} \int_{-\infty}^{\infty} N_{\beta}^2(q) \left[\left(\boldsymbol{\beta}_+^{(+)} \right)^* \times \boldsymbol{\beta}_+^{(+)} - \left(\boldsymbol{\beta}_-^{(+)} \right)^* \times \boldsymbol{\beta}_-^{(+)} \right] d^3q. \quad (15.90)$$

Since

$$\hat{\mathbf{e}}_+^* \times \hat{\mathbf{e}}_+ = -\hat{\mathbf{e}}_-^* \times \hat{\mathbf{e}}_- = i\hat{\mathbf{q}}, \quad (15.91)$$

the photon momentum can be given in terms of the scalar amplitudes of the two helicity eigenstates, viz.,

$$\mathbf{P} = \int_{-\infty}^{\infty} \hbar \mathbf{q} \left[\sum_{s=+,-} \left(\beta_s^{(+)}(\mathbf{q}; t) \right)^* \beta_s^{(+)}(\mathbf{q}; t) \right] d^3 q, \quad (15.92)$$

where use has been made of (15.66) and (15.71). The one-photon momentum hence appears as the quantum mechanical mean value of the photon momentum operator $\hbar \mathbf{q}$, a satisfactory result.

In terms of the mean value of the four-vector momentum operator $\{p^\mu\} = \hbar(q, \mathbf{q}) = \hbar(\omega/c_0, \mathbf{q})$, the contravariant one-photon energy–momentum four-vector

$$\{P^\mu\} = \left(\frac{E}{c_0}, \mathbf{P} \right) \quad (15.93)$$

takes the compact quantum mechanical form

$$\{P^\mu\} = \int_{-\infty}^{\infty} \{p^\mu\} \left[\sum_{s=+,-} \left(\beta_s^{(+)}(\mathbf{q}; t) \right)^* \beta_s^{(+)}(\mathbf{q}; t) \right] d^3 q. \quad (15.94)$$

In the spinor description, where the photon four-vector momentum operator has the block diagonal form

$$[p^\mu] \equiv \begin{pmatrix} \{p^\mu\} (U - \hat{\mathbf{p}} \hat{\mathbf{p}}) & \mathbf{0} \\ \mathbf{0} & \{p^\mu\} (U - \hat{\mathbf{p}} \hat{\mathbf{p}}) \end{pmatrix}, \quad (15.95)$$

the energy–momentum four-vector of the photon is given by

$$\begin{aligned} \{P^\mu\} &= \langle \Phi^{\text{CF}} | [p^\mu] | \Phi^{\text{CF}} \rangle \\ &= \int_{-\infty}^{\infty} (\Phi^{\text{CF}}(\mathbf{q}; t))^{\dagger} \cdot [p^\mu] \cdot \Phi^{\text{CF}}(\mathbf{q}; t) d^3 q \end{aligned} \quad (15.96)$$

in the framework of the complex field theory.

15.5 Complex Field Theory in the Space–Time Domain

15.5.1 Cartesian Photon Spin Operator: Helicity Operator

Let us return to the dynamical equations for the complex field vectors $\beta_+^{(+)}$ and $\beta_-^{(+)}$. In the momentum–time domain these equations are displayed in (15.70). It is easy to transfer these equations to the space–time domain, one just needs to remember the prescription $i\mathbf{q} \Rightarrow \nabla$. A spatial Fourier transformation therefore immediately leads to the following dynamical equations:

$$i\hbar \frac{\partial}{\partial t} \beta_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \hbar \nabla \times \beta_{\pm}^{(+)}(\mathbf{r}, t). \quad (15.97)$$

We now show that the dynamical equations may be written in a suggestive form which in a preliminary manner introduces us to the photon spin concept. We shall realize in Sect. 15.6 that the photon spin concept enters the photon probability current density, and later on in the book more is to be said on the concept. As a starting point we consider the third-rank Levi–Civita tensor $\{\epsilon_{ijk}\}$, for which $\epsilon_{ijk} = +1$ or -1 according to whether indices i, j and k are an even or odd permutation of x, y and z , and $\epsilon_{ijk} = 0$ otherwise. For reasons to become clear shortly, we multiply the Levi–Civita tensor by a factor $\hbar/i$. Next, we form from each of the three Cartesian k -components of $(\hbar/i)\epsilon_{ijk}$ a second-rank 3×3 matrix. We denote the three new matrices by s_k , $k = x, y, z$, and relate the ij th matrix element of s_k to ϵ_{ijk} as follows:

$$(s_k)_{ij} \equiv \frac{\hbar}{i} \epsilon_{ijk}. \quad (15.98)$$

It is now suggested that the s_k 's may be considered as matrix representatives of the three Cartesian components of a photon spin operator $\hat{s}$, i.e.,

$$\hat{s} = (\hat{s}_x, \hat{s}_y, \hat{s}_z) = (s_x, s_y, s_z). \quad (15.99)$$

Below we give some hints that this interpretation might be correct, but first the explicit matrix forms representing the Cartesian components of the photon spin operator are written down. Thus,

$$\hat{s}_x = \frac{\hbar}{i} \{\epsilon_{ijx}\} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad (15.100)$$

$$\hat{s}_y = \frac{\hbar}{i} \{\epsilon_{ijy}\} = \hbar \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad (15.101)$$

$$\hat{s}_z = \frac{\hbar}{i} \{\epsilon_{ijz}\} = \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (15.102)$$

Simple matrix manipulations show that the components of the spin operator satisfy the commutator relations

$$[\hat{s}_i, \hat{s}_j] = i\hbar\epsilon_{ijk}\hat{s}_k, \quad (15.103)$$

which in compact notation can be written

$$\hat{s} \times \hat{s} = i\hbar\hat{s}. \quad (15.104)$$

The set of commutator relations in (15.103) has a form which *defines* an angular momentum operator in quantum mechanics. The Cartesian components of the spin operator all have the eigenvalues 0 and $\pm\hbar$, as the reader may convince himself of.

The operator

$$\hat{s}^2 = \hat{s}_x^2 + \hat{s}_y^2 + \hat{s}_z^2 = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (15.105)$$

which characterizes the squared length of the spin vector quantum mechanically, has the triply degenerate eigenvalue $2\hbar^2$. The results above of course are in agreement with the general consideration for a spin-one particle ($s = 1$), namely

$$eV(\hat{s}^2) = s(s+1)\hbar^2, \quad (15.106)$$

$$eV(\hat{s}_z) = m\hbar, \quad -s \leq m \leq s. \quad (15.107)$$

Let us now demonstrate how the photon spin operator can be introduced in the dynamical equations in (15.97). Thus, if one multiplies the matrix (operator)

$$\hat{\mathbf{s}} \cdot \mathbf{a} = \hat{s}_x a_x + \hat{s}_y a_y + \hat{s}_z a_z = i\hbar \begin{pmatrix} 0 & -a_z & a_y \\ a_z & 0 & -a_x \\ -a_y & a_x & 0 \end{pmatrix} \quad (15.108)$$

from the right with the vector $\mathbf{F}$, one obtains

$$(\hat{\mathbf{s}} \cdot \mathbf{a}) \cdot \mathbf{F} = i\hbar \mathbf{a} \times \mathbf{F}, \quad (15.109)$$

For the arbitrary vector $\mathbf{a}$. The relation in (15.109) is the key we need for the rewriting of the dynamical equations for $\beta_{\pm}^{(+)}(\mathbf{r}, t)$. It appears from the derivation that (15.109) also holds if $\mathbf{a}$ is the differential operator ∇ that is with $\mathbf{F} = \beta_{\pm}^{(+)}$

$$(\hat{\mathbf{s}} \cdot \nabla) \cdot \beta_{\pm}^{(+)}(\mathbf{r}, t) = i\hbar \nabla \times \beta_{\pm}^{(+)}(\mathbf{r}, t) \quad (15.110)$$

A combination of (15.97) and (15.110) leads to the wanted forms

$$i\hbar \frac{\partial}{\partial t} \beta_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \left(\frac{\hat{\mathbf{s}}}{\hbar} \cdot \frac{\hbar}{i} \nabla \right) \cdot \beta_{\pm}^{(+)}(\mathbf{r}, t). \quad (15.111)$$

In the operator on the right side of the double equation above appears an important scalar product between the photon spin and momentum operators. In the momentum representation, where $\hat{\mathbf{p}} = \mathbf{p}$, the projection of the spin operator on the direction of the momentum, i.e.,

$$\hat{h} = \hat{\mathbf{s}} \cdot \frac{\mathbf{p}}{p} \quad (15.112)$$

defines the so-called photon helicity operator. The physical importance of this operator is discussed in Chap. 17, and later on in this book.

The spinor description of photon wave mechanics also can be formulated in the space–time domain. Here the supermatrix Hamiltonian operator is

$$\mathcal{H}(\nabla) = \frac{c_0}{i} \begin{pmatrix} \hat{s} \cdot \nabla & \mathbf{0} \\ \mathbf{0} & -\hat{s} \cdot \nabla \end{pmatrix}, \quad (15.113)$$

and the Schrödinger-like wave equation for the six-component photon wave function

$$\Phi^{\text{CF}}(\mathbf{r}, t) = \begin{pmatrix} \Phi_+^{\text{CF}}(\mathbf{r}, t) \\ \Phi_-^{\text{CF}}(\mathbf{r}, t) \end{pmatrix} = (2\pi)^{3/2} \begin{pmatrix} \beta_+^{(+)}(\mathbf{r}, t) \\ \beta_-^{(+)}(\mathbf{r}, t) \end{pmatrix}, \quad (15.114)$$

which upper and lower parts are composed of positive and negative helicity states, respectively, is

$$i\hbar \frac{\partial}{\partial t} \Phi^{\text{CF}}(\mathbf{r}, t) = \mathcal{H}(\nabla) \cdot \Phi^{\text{CF}}(\mathbf{r}, t) \quad (15.115)$$

in the complex field theory. The normalization of the wave function, viz.,

$$\int_{-\infty}^{\infty} (\Phi^{\text{CF}}(\mathbf{r}, t))^{\dagger} \cdot \Phi^{\text{CF}}(\mathbf{r}, t) d^3r = 1 \quad (15.116)$$

follows from the Parseval–Plancherel identity [(9.56)], and (15.75). The factor $(2\pi)^{3/2}$ introduced in (15.114) is useful because it finally eliminates the conversion factor $(2\pi)^{-3}$ appearing in (9.56).

15.5.2 The Nonlocal Hamilton Operator of the Photon

In the CF theory, the scalar photon wave functions for the two helicity states, $\beta_{\pm}^{(+)}(\mathbf{q}; t)$ satisfy the wave equation in (15.73). By means of the folding theorem, it appears that the space–time wave functions $\beta_{\pm}^{(+)}(\mathbf{r}; t)$ formally fulfil an integro-differential equation of the form

$$i\hbar \frac{\partial}{\partial t} \beta_{\pm}^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathcal{H}(|\mathbf{r} - \mathbf{r}'|) \beta_{\pm}^{(+)}(\mathbf{r}', t) d^3r', \quad (15.117)$$

with a spatially nonlocal and singular real Hamiltonian density operator

$$\mathcal{H}(R) = (2\pi)^{-3} \int_{-\infty}^{\infty} c_0 \hbar q e^{i\mathbf{q} \cdot \mathbf{R}} d^3r. \quad (15.118)$$

Since the Hamilton operator in $\mathbf{q}$ -space, $c_0 \hbar q$, only depends on the magnitude of the wave vector, its Fourier transform is a function of $R = |\mathbf{r} - \mathbf{r}'|$. At this stage it is interesting to compare (15.118) to the action of the nonlocal Landau–Peierls operator $\sqrt{\Delta}$, see (15.20) and (15.21). For $F(\mathbf{q}) = 1$, one has $F(\mathbf{r}) = \delta(\mathbf{r})$, and thus

$$\sqrt{\Delta} \delta(\mathbf{r}) = i \int_{-\infty}^{\infty} q e^{i\mathbf{q} \cdot \mathbf{r}} \frac{d^3q}{(2\pi)^3}. \quad (15.119)$$

A comparison of (15.118) and (15.119) then immediately shows that

$$\mathcal{H}(R) = -i c_0 \hbar \sqrt{\Delta} \delta(R). \quad (15.120)$$

Using spherical coordinates in $\mathbf{q}$ -space, and with the polar axis along the $\mathbf{R}$ -direction, it is easy to determine the singular structure of $\mathcal{H}$ in (15.118). After having carried out the trivial angular integrations one has

$$\mathcal{H}(R) = \frac{c_0 \hbar}{4\pi^2 i R} \int_0^\infty q^2 \left(e^{iqR} - e^{-iqR} \right) dq. \quad (15.121)$$

The remaining singular integral is conveniently expressed in terms of the positive wave number part of the Dirac delta function, viz.,

$$\delta^{(+)}(R) = (2\pi)^{-1} \int_0^\infty e^{iqR} dq. \quad (15.122)$$

The slight difference in the definition of $\delta^{(+)}$ used in (15.44) and (15.122) is useful in connection with the plane-wave, $\exp[i(\mathbf{q} \cdot \mathbf{R} - \omega\tau)]$, Fourier decomposition of the various fields. Since

$$\frac{d^2}{dR^2} \delta^{(+)}(R) = - \int_0^\infty q^2 e^{iqR} \frac{dq}{2\pi}, \quad (15.123)$$

the Hamiltonian density may finally be given in the form

$$\mathcal{H}(R) = \frac{i c_0 \hbar}{2\pi R} \frac{d^2}{dR^2} \left[\delta^{(+)}(R) - \left(\delta^{(+)}(R) \right)^* \right]. \quad (15.124)$$

The complex conjugate of the positive wave-number delta function, $(\delta^{(+)}(R))^*$, equals the negative wave-number part of $\delta(R)$, defined by

$$\delta^{(-)}(R) = (2\pi)^{-1} \int_{-\infty}^0 e^{iqR} dq, \quad (15.125)$$

as the reader may prove to herself. Because

$$\delta^\pm(R) = \frac{1}{2} \left(\delta(R) \pm \frac{i}{\pi} P \frac{1}{R} \right), \quad (15.126)$$

cf. (15.42) [with $\tau \Rightarrow -R$], the photon Hamiltonian density can also be expressed in compact notation as follows:

$$\mathcal{H}(R) = -\frac{c_0 \hbar}{2\pi^2 R} \frac{d^2}{dR^2} \left(P \frac{1}{R} \right). \quad (15.127)$$

15.6 Photon Probability Current Density and the Associated Operator

In free space, photons cannot be created nor destroyed, and therefore it is a priori obvious that the photon probability density must satisfy a local conservation law. Furthermore, due to the fact that the wave functions of the positive and negative helicity states do not couple in vacuum, each of the species satisfies their own local conservation law. When the dynamical equations for the upper (Φ_+^{CF}) and lower (Φ_-^{CF}) parts of the photon spinor are utilized in a rewriting of the time derivatives of the species' probability current densities explicit expressions emerge for the probability current densities of the two helicity states.

To establish the local probability conservation laws for the two species one starts from the relations

$$\frac{\partial}{\partial t} \left[\Phi_{\pm}^{\text{CF}} \cdot (\Phi_{\pm}^{\text{CF}})^* \right] = (\Phi_{\pm}^{\text{CF}})^* \cdot \frac{\partial}{\partial t} \Phi_{\pm}^{\text{CF}} + \Phi_{\pm}^{\text{CF}} \cdot \frac{\partial}{\partial t} (\Phi_{\pm}^{\text{CF}})^*, \quad (15.128)$$

and eliminates thereafter the time derivatives on the right side by means of the dynamical equations

$$\frac{\partial}{\partial t} \Phi_{\pm}^{\text{CF}} = \mp i c_0 \nabla \times \Phi_{\pm}^{\text{CF}}, \quad (15.129)$$

and their complex conjugates

$$\frac{\partial}{\partial t} (\Phi_{\pm}^{\text{CF}})^* = \pm i c_0 \nabla \times (\Phi_{\pm}^{\text{CF}})^*. \quad (15.130)$$

Thus, one obtains

$$\frac{\partial}{\partial t} \left[\Phi_{\pm}^{\text{CF}} \cdot (\Phi_{\pm}^{\text{CF}})^* \right] = \pm i c_0 \Phi_{\pm}^{\text{CF}} \cdot \nabla \times (\Phi_{\pm}^{\text{CF}})^* \mp i c_0 (\Phi_{\pm}^{\text{CF}})^* \cdot \nabla \times \Phi_{\pm}^{\text{CF}}, \quad (15.131)$$

or equivalently

$$\frac{\partial}{\partial t} \left[\Phi_{\pm}^{\text{CF}} \cdot (\Phi_{\pm}^{\text{CF}})^* \right] = \mp i c_0 \nabla \cdot \left[\Phi_{\pm}^{\text{CF}} \times (\Phi_{\pm}^{\text{CF}})^* \right]. \quad (15.132)$$

It appears from the equations in (15.132) that the probability densities for the positive (N_+^{CF}) and negative (N_-^{CF}) helicity states, viz.,

$$N_{\pm}^{\text{CF}}(\mathbf{r}, t) = \Phi_{\pm}^{\text{CF}}(\mathbf{r}, t) \cdot (\Phi_{\pm}^{\text{CF}}(\mathbf{r}, t))^* \quad (15.133)$$

satisfy the separate local conservation laws

$$\nabla \cdot \mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) + \frac{\partial}{\partial t} N_{\pm}^{\text{CF}}(\mathbf{r}, t) = 0, \quad (15.134)$$

where

$$\mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) = \pm i c_0 \boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t) \times (\boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t))^* \quad (15.135)$$

may be interpreted as the probability current densities associated with the two helicity states. Note that divergence-free parts can be added to $\mathbf{I}_{+}^{\text{CF}}$ and $\mathbf{I}_{-}^{\text{CF}}$ without changing the conservation laws. The possible importance of such a freedom is not investigated here. By addition of the conservation laws for the helicity species we of course obtain a conservation law for the total photon probability density, namely

$$\nabla \cdot \mathbf{I}^{\text{CF}}(\mathbf{r}, t) + \frac{\partial}{\partial t} N^{\text{CF}}(\mathbf{r}, t) = 0, \quad (15.136)$$

where $N^{\text{CF}} = N_{+}^{\text{CF}} + N_{-}^{\text{CF}}$ and $\mathbf{I}^{\text{CF}} = \mathbf{I}_{+}^{\text{CF}} + \mathbf{I}_{-}^{\text{CF}}$. For plane-wave photons (normalized over a finite length, though) the probability densities are space and time independent, and the wave functions for the two helicity eigenstates

$$\boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t) = \sqrt{N_{\pm}^{\text{CF}}} \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) \exp[i(\mathbf{q} \cdot \mathbf{r} - \omega t)] \quad (15.137)$$

have the associated space-time constant probability current densities

$$\mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) = N_{\pm}^{\text{CF}} c_0 \hat{\mathbf{q}}, \quad (15.138)$$

as the reader readily may show using the relations

$$\hat{\mathbf{e}}_{\pm} \times \hat{\mathbf{e}}_{\pm}^* = \mp i \hat{\mathbf{q}}. \quad (15.139)$$

As expected, it appears from (15.138) that the probability current densities of the positive- and negative-helicity states both are in the direction of the photon momentum.

By means of (15.109) [with $\mathbf{a} = (\boldsymbol{\Phi}_{\pm}^{\text{CF}})^*$ and $\mathbf{F} = \boldsymbol{\Phi}_{\pm}^{\text{CF}}$] the expressions for the current densities easily can be written in spinor notation. Thus,

$$\mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) = \pm c_0 \left[\frac{\hat{\mathbf{s}}}{\hbar} \cdot (\boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t))^* \right] \cdot \boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t), \quad (15.140)$$

or equivalently

$$\mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) = \pm c_0 (\boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t))^{\dagger} \cdot \frac{\hat{\mathbf{s}}}{\hbar} \cdot \boldsymbol{\Phi}_{\pm}^{\text{CF}}(\mathbf{r}, t). \quad (15.141)$$

If one introduces the Hermitian photon probability current density operators for the positive and negative helicities, namely

$$\hat{\mathbf{i}}_{\pm}^{\text{CF}} = \pm \frac{c_0}{\hbar} \delta(\mathbf{r} - \mathbf{r}') \hat{\mathbf{s}}, \quad (15.142)$$

the probability current densities may be obtained as quantum mechanical mean values of $\hat{\mathbf{i}}_{\pm}^{\text{CF}}$, i.e.,

$$\mathbf{I}_{\pm}^{\text{CF}}(\mathbf{r}, t) = \int_{-\infty}^{\infty} (\boldsymbol{\Phi}^{\text{CF}}(\mathbf{r}', t))^{\dagger} \cdot \hat{\mathbf{i}}_{\pm}^{\text{CF}}(\mathbf{r} - \mathbf{r}') \cdot \boldsymbol{\Phi}^{\text{CF}}(\mathbf{r}', t) d^3 r'. \quad (15.143)$$

The matrix representation of $\hat{\mathbf{i}}_{\pm}^{\text{CF}}$ follows from that of $\hat{\mathbf{s}}$ (15.98).

15.7 The Nonlocal Relation Between Field Vectors and Photon Wave Function

It appears from the calculations in Sect. 15.4.4 that in order for the photon energy and momentum to take the familiar quantum mechanical forms the normalization constant $N_{\beta}(q)$ necessarily must depend on the magnitude of the wave vector; see (15.66). Such a dependence implies that the relation between the vectorial photon wave functions, $\boldsymbol{\beta}_{\pm}^{(+)}$, and the complex electromagnetic field vectors takes a spatially nonlocal form in the space–time domain. Application of the convolution theorem to (15.65) immediately gives

$$\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} k(|\mathbf{r} - \mathbf{r}'|) \left(\mathbf{e}_{\text{T}}^{(+)}(\mathbf{r}', t) \pm i \mathbf{b}^{(+)}(\mathbf{r}', t) \right) d^3 r', \quad (15.144)$$

where

$$k(|\mathbf{R}|) = \frac{1}{2} (2\pi)^{-9/2} \left(\frac{\epsilon_0}{\hbar c_0} \right)^{1/2} \int_{-\infty}^{\infty} q^{-1/2} e^{i\mathbf{q} \cdot \mathbf{R}} d^3 q. \quad (15.145)$$

The range of the nonlocal connection follows from an explicit evaluation of the integral in (15.145). It appears obvious to carry out the integration in spherical coordinates with the polar axis along the $\mathbf{R}$ -direction. The integrations over azimuth and polar angles are easily done, and with the substitution $x = qR$ one thereafter obtains

$$\int_{-\infty}^{\infty} q^{-1/2} e^{i\mathbf{q} \cdot \mathbf{R}} d^3 q = \frac{4\pi}{R^{5/2}} \int_{-\infty}^{\infty} x^{1/2} \sin x dx. \quad (15.146)$$

Strictly speaking the integral over x does not exist because the integral oscillates infinitely rapid between plus and minus infinity for $qR = x \rightarrow \infty$. From a physical point of view this problem itself is not so serious since infinitely high wave numbers (q) do not appear in photon–matter interactions. Without loss of generality one may, therefore, regularize the integral by introducing an exponential factor $\exp(-\epsilon x)$, $\epsilon > 0$, under the integral sign. After the integration has been carried out one takes the limit $\epsilon \rightarrow 0$. Thus, we use the formula [290]

$$\int_0^\infty x^{\mu-1} e^{-\epsilon x} \sin x dx = \frac{\Gamma(\mu)}{(1 + \epsilon^2)^{\mu/2}} \sin \left[\mu \arctan \left(\frac{1}{\epsilon} \right) \right], \quad (15.147)$$

where $\Gamma(\mu)$ is the gamma function. For $\mu = 3/2$, the integral in (15.147) equals $\sqrt{2\pi}/4$ in the limit $\epsilon \rightarrow 0$. Altogether, we hence obtain the following expression for the function $k(|\mathbf{R}|)$ describing the nonlocal relation between the vectorial wave functions of the two helicity states and the complex electromagnetic field vectors:

$$k(|\mathbf{R}|) = \frac{1}{4} (2\pi)^{-3} \sqrt{\frac{\epsilon_0}{\hbar c_0}} R^{-5/2}. \quad (15.148)$$

It appears from (15.144) and (15.148) that even if one could localize the (analytical part of the) electromagnetic field at a given point in space (at a given time) the associated photon wave function would spread out in the neighborhood of this point with a fall-off characterized by $R^{-5/2}$ in the framework of the complex field theory. It is not possible to localize the electromagnetic field completely because this would require the field energy density to become infinitely large in the point of localization.

With the help of (15.83) and (15.84) and the convolution theorem, the reader may show to herself that the inverse relation to (15.144), viz.,

$$e_{\mathbf{T}}^{(+)}(\mathbf{r}, t) \pm i c_0 \mathbf{b}^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} k^{-1}(|\mathbf{r} - \mathbf{r}'|) \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{r}', t) d^3 r' \quad (15.149)$$

has the kernel

$$k^{-1}(|\mathbf{R}|) = 2(2\pi)^{-3/2} \left(\frac{\hbar c_0}{\epsilon_0} \right)^{1/2} \int_{-\infty}^{\infty} q^{1/2} e^{i\mathbf{q} \cdot \mathbf{R}} d^3 q. \quad (15.150)$$

A regularization procedure analogous to the one discussed above but now with $\mu = 5/2$ in (15.147) leads to

$$k^{-1}(|\mathbf{R}|) = -\frac{3}{2} \left(\frac{\hbar c_0}{\epsilon_0} \right)^{1/2} R^{-7/2}. \quad (15.151)$$

In a sense, the result in (15.151) underlines the remarks given below (15.148). Thus, even if one was able to localize the photon completely in space, an electromagnetic field would still be present in the surroundings of the point of localization, and the complex field vectors for the two helicity states would decay in space as $R^{-7/2}$. The localization profiles given by $k(|\mathbf{R}|)$ and $k^{-1}(|\mathbf{R}|)$ are not the same, but interestingly enough the square root of the products $R^{-5/2} R^{-7/2}$ just gives the R^{-3} -dependence so characteristic for near-field electrodynamics.

The two kernels $k(|\mathbf{R}|)$ and $k^{-1}(|\mathbf{R}|)$ are the reciprocal of each other in the generalized sense that

$$\int_{-\infty}^{\infty} k(|\mathbf{r} - \mathbf{r}''|) k^{-1}(|\mathbf{r}'' - \mathbf{r}'|) d^3 r'' = \delta(\mathbf{r} - \mathbf{r}'). \quad (15.152)$$

In order to prove this we insert the expansions in (15.145) and (15.150) into the left side of (15.152), denoting the integration variables in the reciprocal space by $\mathbf{q}$ and $\mathbf{Q}$, respectively. By interchange of the $\mathbf{r}''$ -integration and the $(\mathbf{q}, \mathbf{Q})$ -integrations one obtains

$$\begin{aligned}
 & \int_{-\infty}^{\infty} k(|\mathbf{r} - \mathbf{r}''|) k^{-1}(|\mathbf{r}'' - \mathbf{r}'|) d^3 r'' \\
 &= (2\pi)^{-6} \int_{-\infty}^{\infty} \left(\frac{Q}{q} \right)^{1/2} e^{i(\mathbf{Q} \cdot \mathbf{r} - \mathbf{q} \cdot \mathbf{r}')} e^{i(\mathbf{q} - \mathbf{Q}) \cdot \mathbf{r}''} d^3 r'' d^3 Q d^3 q \\
 &= (2\pi)^{-3} \int_{-\infty}^{\infty} \left(\frac{Q}{q} \right)^{1/2} e^{i(\mathbf{Q} \cdot \mathbf{r} - \mathbf{q} \cdot \mathbf{r}')} \delta(\mathbf{Q} - \mathbf{q}) d^3 Q d^3 q \\
 &= (2\pi)^{-3} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} d^3 q. \tag{15.153}
 \end{aligned}$$

The last integral is just the plane-wave expansion of the Dirac delta function $\delta(\mathbf{r} - \mathbf{r}')$, and this concludes our proof of (15.152).

Chapter 16

Photon Wave Mechanics: Energy Wave Function and Four-Potential Theories

On the basis of the electromagnetic field vectors a photon wave function can be constructed in various manners. From a physical point of view different choices are in a sense equivalent provided they satisfy the free-space Maxwell equations. In order to make the quantum mechanical description of all, massive and non-massive, particles uniform certain choices are more attractive than others, however. In the complex field theory discussed in Chap. 15, the vectorial wave functions for the two photon helicity states are related to the electromagnetic field in a manner which is spatially nonlocal but timely local. This asymmetry between the space and time connections makes the complex field theory less attractive from a relativistic point of view. It appears from the analysis in Sect. 15.7 that the nonlocality in the spatial connection between field and wave function originates in the fact that the normalization constant $N_\beta(q)$ depends on the photon wave number. In this chapter we shall study two choices for a photon wave function which both connect the wave function and the electromagnetic field locally in space and time. From a relativistic point of view both choices are quite satisfactory.

16.1 Photon Energy Wave Function Formalism

16.1.1 Riemann–Silberstein Approach to Classical Electromagnetics in Free Space

In the free-space Maxwell equations given in (15.8)–(15.10), the two transverse and real vector fields $\mathbf{E}_T(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ appear. The information in the Maxwell equations can be expressed in a more compact form by introduction of the complex Riemann–Silberstein vector

$$\mathbf{F}_+(\mathbf{r}, t) \equiv \sqrt{\frac{\epsilon_0}{2}} (\mathbf{E}_T(\mathbf{r}, t) + i c_0 \mathbf{B}(\mathbf{r}, t)). \quad (16.1)$$

Since the free-space Maxwell equations are homogeneous the factor $(\epsilon_0/2)^{1/2}$ plays no essential role at this stage. If one multiplies (15.9) by $i c_0$ and thereafter adds the

resulting equation to (15.8) it is easily realized that $\mathbf{F}_+(\mathbf{r}, t)$ satisfies the partial differential equation

$$\nabla \times \mathbf{F}_+(\mathbf{r}, t) = \frac{i}{c_0} \frac{\partial}{\partial t} \mathbf{F}_+(\mathbf{r}, t). \quad (16.2)$$

The relations in (15.10) further show that $\mathbf{F}_+(\mathbf{r}, t)$ is a transverse vector field, i.e.,

$$\nabla \cdot \mathbf{F}_+(\mathbf{r}, t) = 0. \quad (16.3)$$

In terms of the Riemann–Silberstein vector in (16.1), the full content of the free-space Maxwell equations is displayed in (16.2) and (16.3). In preparation of the photon wave mechanical description a second complex Riemann–Silberstein vector $\mathbf{F}_-(\mathbf{r}, t)$ is defined via

$$\mathbf{F}_-(\mathbf{r}, t) \equiv \sqrt{\frac{\epsilon_0}{2}} (\mathbf{E}_T(\mathbf{r}, t) - i c_0 \mathbf{B}(\mathbf{r}, t)). \quad (16.4)$$

Since

$$\mathbf{F}_-(\mathbf{r}, t) = \mathbf{F}_+^*(\mathbf{r}, t), \quad (16.5)$$

complex conjugation of (16.2) and (16.3) immediately shows that the dynamical equations for $\mathbf{F}_-(\mathbf{r}, t)$ are

$$\nabla \times \mathbf{F}_-(\mathbf{r}, t) = -\frac{i}{c_0} \frac{\partial}{\partial t} \mathbf{F}_-(\mathbf{r}, t), \quad (16.6)$$

and

$$\nabla \cdot \mathbf{F}_-(\mathbf{r}, t) = 0. \quad (16.7)$$

In compact form we write (16.2), (16.3), (16.6), and (16.7) as follows

$$i \frac{\partial}{\partial t} \mathbf{F}_\pm(\mathbf{r}, t) = \pm c_0 \nabla \times \mathbf{F}_\pm(\mathbf{r}, t), \quad (16.8)$$

$$\nabla \cdot \mathbf{F}_\pm(\mathbf{r}, t) = 0. \quad (16.9)$$

For the purposes of classical electrodynamics one may restrict oneself to use either $\mathbf{F}_+(\mathbf{r}, t)$ or $\mathbf{F}_-(\mathbf{r}, t)$.

As shown below, the energy, momentum and angular momentum of the transverse electromagnetic field can be represented in terms of bilinear expressions constructed from $\mathbf{F}_+$, $\mathbf{F}_-$ or both. Since

$$E_T^2 + c_0^2 \mathbf{B}^2 = (\mathbf{E}_T + i c_0 \mathbf{B}) \cdot (\mathbf{E}_T - i c_0 \mathbf{B}), \quad (16.10)$$

it follows that the energy in the transverse field (9.70) may be expressed in the mixed form

$$H_{\text{trans}} = \int_{-\infty}^{\infty} \mathbf{F}_+(\mathbf{r}, t) \cdot \mathbf{F}_-(\mathbf{r}, t) d^3r. \quad (16.11)$$

Alternative forms containing either $\mathbf{F}_+$ or $\mathbf{F}_-$ are obtained using (16.5). Thus,

$$H_{\text{trans}} = \int_{-\infty}^{\infty} \mathbf{F}_+^*(\mathbf{r}, t) \cdot \mathbf{F}_+(\mathbf{r}, t) d^3r = \int_{-\infty}^{\infty} \mathbf{F}_-^*(\mathbf{r}, t) \cdot \mathbf{F}_-(\mathbf{r}, t) d^3r. \quad (16.12)$$

To express the momentum (9.81) and angular momentum (9.95) of the transverse field in terms of the complex Riemann–Silberstein vectors one first solves (16.1) and (16.4) with respect to $\mathbf{E}_T$ and $\mathbf{B}$. From the solution

$$\mathbf{E}_T(\mathbf{r}, t) = \frac{1}{\sqrt{2\epsilon_0}} (\mathbf{F}_+(\mathbf{r}, t) + \mathbf{F}_-(\mathbf{r}, t)), \quad (16.13)$$

$$\mathbf{B}(\mathbf{r}, t) = \frac{1}{ic_0} \frac{1}{\sqrt{2\epsilon_0}} (\mathbf{F}_+(\mathbf{r}, t) - \mathbf{F}_-(\mathbf{r}, t)), \quad (16.14)$$

one obtains

$$\epsilon_0 \mathbf{E}_T \times \mathbf{B} = \frac{1}{2ic_0} (\mathbf{F}_- \times \mathbf{F}_+ - \mathbf{F}_+ \times \mathbf{F}_-) = \frac{1}{ic_0} \mathbf{F}_- \times \mathbf{F}_+, \quad (16.15)$$

and consequently the following expression for the momentum

$$\mathbf{P}_{\text{trans}} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{F}_-(\mathbf{r}, t) \times \mathbf{F}_+(\mathbf{r}, t) d^3r. \quad (16.16)$$

Alternative expressions read

$$\mathbf{P}_{\text{trans}} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{F}_+^*(\mathbf{r}, t) \times \mathbf{F}_+(\mathbf{r}, t) d^3r = \frac{i}{c_0} \int_{-\infty}^{\infty} \mathbf{F}_-^*(\mathbf{r}, t) \times \mathbf{F}_-(\mathbf{r}, t) d^3r. \quad (16.17)$$

The angular momentum of the transverse field may be given as

$$\mathbf{I}_{\text{trans}} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{r} \times (\mathbf{F}_-(\mathbf{r}, t) \times \mathbf{F}_+(\mathbf{r}, t)) d^3r, \quad (16.18)$$

or in forms containing solely $\mathbf{F}_-$ or $\mathbf{F}_+$.

16.1.2 Dynamical Equation for the Photon Energy Wave Function

As a preparation to the introduction of the photon energy wave function in direct space we start from the positive-frequency parts of the Riemann–Silberstein vectors

in (16.1) and (16.4), i.e.,

$$\mathbf{F}_{\pm}^{(+)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(\mathbf{E}_{\text{T}}^{(+)}(\mathbf{r}, t) \pm i c_0 \mathbf{B}^{(+)}(\mathbf{r}, t) \right). \quad (16.19)$$

In free space, the analytical parts of the electric and magnetic fields satisfy the dynamical equations

$$\nabla \times \mathbf{E}_{\text{T}}^{(+)}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}^{(+)}(\mathbf{r}, t), \quad (16.20)$$

$$\nabla \times \mathbf{B}^{(+)}(\mathbf{r}, t) = \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{E}_{\text{T}}^{(+)}(\mathbf{r}, t), \quad (16.21)$$

and the transversality conditions

$$\nabla \cdot \mathbf{E}_{\text{T}}^{(+)}(\mathbf{r}, t) = \nabla \cdot \mathbf{B}^{(+)}(\mathbf{r}, t) = 0. \quad (16.22)$$

The correctness of these equations, which are form-identical to the free-space Maxwell equations in (15.8)–(15.10), is obvious since the sets (15.67)–(15.69) and (16.20)–(16.22) are just the spatial Fourier transforms of each other. The homogeneity of the dynamical equations implies that from a given solution $(\mathbf{E}_{\text{T}}^{(+)}, \mathbf{B}^{(+)})$ other solutions can be obtained by multiplying this solution with an arbitrary constant. The particular solution of relevance for one-photon wave mechanics we denote by $\mathbf{e}_{\text{T}}^{(+)}$, $\mathbf{b}^{(+)}$, cf. the notation adopted in Sect. 15.4.2. The related positive-frequency Riemann–Silberstein vectors, which we denote by $\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$, are

$$\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(\mathbf{e}_{\text{T}}^{(+)}(\mathbf{r}, t) \pm i c_0 \mathbf{b}^{(+)}(\mathbf{r}, t) \right). \quad (16.23)$$

It appears from (16.8) that the $\mathbf{f}_{\pm}^{(+)}$'s satisfy the dynamical equations

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \hbar \nabla \times \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t). \quad (16.24)$$

Since these are form-identical to the dynamical equations for the complex field vectors, $\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{r}, t)$, (16.24) can be rewritten as follows:

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \left(\frac{\hat{\mathbf{s}}}{\hbar} \cdot \frac{\hbar}{i} \nabla \right) \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t), \quad (16.25)$$

cf. (15.97) and (15.111). As in the complex field theory, it is useful to work with a spinor description in the photon energy wave function formalism. The states composed of positive ($\mathbf{f}_{+}^{(+)}$) and negative ($\mathbf{f}_{-}^{(+)}$) helicity components thus are combined to a six-component photon energy wave function

$$\Phi(\mathbf{r}, t) = \begin{pmatrix} f_+^{(+)}(\mathbf{r}, t) \\ f_-^{(+)}(\mathbf{r}, t) \end{pmatrix}. \quad (16.26)$$

The photon wave function $\Phi(\mathbf{r}, t)$ satisfies the Schrödinger-like wave equation

$$i\hbar \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) = \mathcal{H}(\nabla) \cdot \Phi(\mathbf{r}, t), \quad (16.27)$$

where $\mathcal{H}(\nabla)$ is the supermatrix Hamiltonian operator introduced in (15.113).

The object $\Phi(\mathbf{r}, t)$ is not just called the photon wave function but the photon *energy* wave function because

$$\int_{-\infty}^{\infty} \Phi^+(\mathbf{r}, t) \cdot \Phi(\mathbf{r}, t) d^3r = E, \quad (16.28)$$

where E is the energy of the photon. What do we mean by saying that E is the photon energy? According to (16.23) the photon is associated with the analytical classical field vectors ($e_T^{(+)}(\mathbf{r}, t)$, $b^{(+)}(\mathbf{r}, t)$), and as we shall prove below, E is precisely the energy in a classical electromagnetic field with the electric and magnetic field strengths $e_T(\mathbf{r}, t)$ and $b(\mathbf{r}, t)$. Although a deeper analysis of the spatial localization problem for the photon is needed, we may tentatively say that $\Phi^+(\mathbf{r}, t) \cdot \Phi(\mathbf{r}, t) d^3r$ gives the probability that the photon energy is located in the infinitesimal volume d^3r around $\mathbf{r}$ at time t . If one holds the point of view that the photon *is* its energy, the energy wave function formalism constitutes a proper framework for a first-quantized theory of the photon.

In order to prove that E (16.28) equals the energy in the classical electromagnetic field, is is convenient to introduce the negative-frequency (superscript $(-)$) Riemann–Silberstein vectors

$$f_{\pm}^{(-)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(e_T^{(-)}(\mathbf{r}, t) \pm ic_0 b^{(-)}(\mathbf{r}, t) \right). \quad (16.29)$$

In Sect. 16.1.1, it was shown that the energy in the transverse (here free) field can be expressed in the form given in (16.11). In the one-photon case we therefore have

$$H_{\text{trans}} = \int_{-\infty}^{\infty} \left(f_+^{(+)} + f_+^{(-)} \right) \cdot \left(f_-^{(+)} + f_-^{(-)} \right) d^3r. \quad (16.30)$$

In order to relate H_{trans} to the one-photon energy (E), which is build exclusively from positive-frequency field components, we now seek to eliminate the $f_{\pm}^{(-)}$'s from (16.30). Since the quantities $e_T(\mathbf{r}, t)$ and $b(\mathbf{r}, t)$ are both real one must have $e_T^{(-)}(\mathbf{r}, t) = [e_T^{(+)}(\mathbf{r}, t)]^*$ and $b^{(-)}(\mathbf{r}, t) = [b^{(+)}(\mathbf{r}, t)]^*$, cf. (15.30). In turn this implies that

$$f_{\pm}^{(-)}(\mathbf{r}, t) = \left[f_{\mp}^{(+)}(\mathbf{r}, t) \right]^*, \quad (16.31)$$

as the reader may readily show. The results in (16.31) allows one to remove the negative-frequency components from (16.30). By insertion of (16.26) and its Hermitian conjugate into (16.28) one obtains

$$E = \int_{-\infty}^{\infty} \left[(f_+^{(+)})^* \cdot f_+^{(+)} + (f_-^{(+)})^* \cdot f_-^{(+)} \right] d^3r. \quad (16.32)$$

A combination of (16.30)–(16.32) next shows that

$$H_{\text{trans}} = E + \Delta, \quad (16.33)$$

where

$$\Delta = \int_{-\infty}^{\infty} f_+^{(+)} \cdot f_-^{(+)} d^3r + c.c. \quad (16.34)$$

Let us finally prove that $\Delta = 0$. Since

$$\begin{aligned} \int_{-\infty}^{\infty} f_+^{(+)}(\mathbf{r}, t) \cdot f_-^{(+)}(\mathbf{r}, t) d^3r &= (2\pi)^{-3} \int_{-\infty}^{\infty} f_+^{(+)}(\mathbf{q}; t) \cdot f_-^{(+)}(-\mathbf{q}; t) d^3q \\ &= (2\pi)^{-3} \int_{-\infty}^{\infty} f_+^{(+)}(\mathbf{q}; t) f_-^{(+)}(-\mathbf{q}; t) \hat{\mathbf{e}}_+(\hat{\mathbf{q}}) \cdot \hat{\mathbf{e}}_-(-\hat{\mathbf{q}}) d^3q, \end{aligned} \quad (16.35)$$

cf. the ansatz in (15.71) (and the analysis in the next subsection), one obtains $\Delta = 0$, provided

$$\hat{\mathbf{e}}_+(\hat{\mathbf{q}}) \cdot \hat{\mathbf{e}}_-(-\hat{\mathbf{q}}) = 0. \quad (16.36)$$

Equation (16.36) is correct since $\hat{\mathbf{e}}_-(-\hat{\mathbf{q}})$ equals $\hat{\mathbf{e}}_+(\hat{\mathbf{q}})$ up to an overall phase factor and $\hat{\mathbf{e}}_+(\hat{\mathbf{q}}) \cdot \hat{\mathbf{e}}_+(\hat{\mathbf{q}}) = 0$. In conclusion, I thus have proved that $H_{\text{trans}} = E$, as promised. A photon once introduced in empty space never disappears. This implies that

$$\frac{d}{dt} \int_{-\infty}^{\infty} \Phi^+(\mathbf{r}, t) \cdot \Phi(\mathbf{r}, t) d^3r = 0, \quad (16.37)$$

a result which the reader may prove to himself follows from the dynamical equations in (16.24). Since $E = H_{\text{trans}}$, (16.37) is a direct consequence of the fact that the electromagnetic energy in free space is a conserved quantity.

16.1.3 Quantum Mechanical Mean Value of the Photon Energy–Momentum Operator in Reciprocal Space

In the previous subsection, the one-photon energy was represented in the form (see (16.32))

$$E = \sum_{s=+,-} \int_{-\infty}^{\infty} \left| f_s^{(+)}(\mathbf{r}, t) \right|^2 d^3r. \quad (16.38)$$

Further insight into the structure of this expression may be obtained by expressing the positive-frequency Riemann–Silberstein vectors as superpositions of plane

waves of the entire $\mathbf{q}$ -domain, i.e.,

$$\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = (2\pi)^{-3} \int_{-\infty}^{\infty} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}, c_0 q) e^{i(\mathbf{q} \cdot \mathbf{r} - c_0 q t)} d^3 q, \quad (16.39)$$

where $\omega = c_0 q > 0$. By means of the Parseval–Plancherel relation (9.56), and the fact $|\exp(-i c_0 q t)| = 1$, it appears that the photon energy can be expressed as

$$E = (2\pi)^{-3} \sum_{s=+,-} \int_{-\infty}^{\infty} \left| \mathbf{f}_s^{(+)}(\mathbf{q}, c_0 q) \right|^2 d^3 q. \quad (16.40)$$

The form-identity of the dynamical equations for the complex field vectors, $\boldsymbol{\beta}_{\pm}^{(+)}$, and the Riemann–Silberstein vectors, $\mathbf{f}_{\pm}^{(+)}$, tells us that it is possible to make the ansatz's

$$\mathbf{f}_{\pm}^{(+)}(\mathbf{q}, c_0 q) = f_{\pm}^{(+)}(\mathbf{q}, c_0 q) \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}). \quad (16.41)$$

By inserting (16.41) and its complex conjugate into (16.40), and utilizing (15.55), one obtains

$$E = (2\pi)^{-3} \sum_{s=+,-} \int_{-\infty}^{\infty} \left| f_s^{(+)}(\mathbf{q}, c_0 q) \right|^2 d^3 q. \quad (16.42)$$

or equivalently

$$E = \frac{1}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \hbar \omega \left| f_s^{(+)}(\mathbf{q}, c_0 q) \right|^2 \frac{d^3 q}{(2\pi)^3 q}. \quad (16.43)$$

As we shall realize in Sect. 16.1.4, (16.43) has a clear relativistic interpretation. At this point it is useful to take

$$g_{\pm}(\mathbf{p}) \equiv (2\pi\hbar)^{-3/2} (c_0 p)^{-1/2} f_{\pm}^{(+)}\left(\frac{\mathbf{p}}{\hbar}, \frac{c_0 p}{\hbar}\right) \quad (16.44)$$

as the time independent scalar energy wave functions for the two photon helicity states in the momentum representation. The related time dependent wave functions are given by

$$g_{\pm}(\mathbf{p}; t) = g_{\pm}(\mathbf{p}) \exp(-i c_0 p t / \hbar). \quad (16.45)$$

In terms of the $g_{\pm}(\mathbf{p}; t)$'s the one-photon energy takes the familiar quantum mechanical mean value form

$$E = \sum_{s=+,-} \int_{-\infty}^{\infty} g_s^*(\mathbf{p}; t) c_0 p g_s(\mathbf{p}; t) d^3 p. \quad (16.46)$$

In spinor notation the photon energy wave function is given by

$$\boldsymbol{\Phi}(\mathbf{p}; t) = \begin{pmatrix} g_+(\mathbf{p}, t) \hat{\mathbf{e}}_+(\hat{\mathbf{p}}) \\ g_-(\mathbf{p}, t) \hat{\mathbf{e}}_-(\hat{\mathbf{p}}) \end{pmatrix} \quad (16.47)$$

in the momentum representation. Although $\Phi(\mathbf{r}, t)$ (16.26) and $\Phi(\mathbf{p}; t)$ in a sense represent the photon wave function in the space and momentum representations, the two spinors do not form a pair of Fourier transforms. The reason for this stems from the presence of the scaling factor $(c_0 p)^{-1/2}$ in (16.44). The normalization of the one-photon state is expressed as

$$\int_{-\infty}^{\infty} \Phi^+(\mathbf{p}; t) \cdot \Phi(\mathbf{p}; t) d^3 p = 1. \quad (16.48)$$

Let us now turn our attention from the photon energy to the photon momentum. It appears from (16.17) that the momentum of the classical electromagnetic field associated with a single photon is given by

$$\mathbf{P}_{\text{trans}} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \left[(\mathbf{f}_+^{(+)*} + (\mathbf{f}_+^{(-)})^* \right] \times \left[\mathbf{f}_+^{(+)} + \mathbf{f}_+^{(-)} \right] d^3 r. \quad (16.49)$$

With the help of (16.31) the negative-frequency parts of the Riemann–Silberstein vectors can be eliminated, and the transverse field momentum hereafter expressed as follows:

$$\mathbf{P}_{\text{trans}} = \mathbf{P} + \mathbf{\Delta}, \quad (16.50)$$

where

$$\mathbf{P} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \left[(\mathbf{f}_+^{(+)*} \times \mathbf{f}_+^{(+)} - (\mathbf{f}_-^{(+)*} \times \mathbf{f}_-^{(+)}) \right] d^3 r, \quad (16.51)$$

and

$$\mathbf{\Delta} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{f}_-^{(+)} \times \mathbf{f}_+^{(+)} d^3 r + c.c. \quad (16.52)$$

To determine the first integral in the expression for $\mathbf{\Delta}$, the integral is transferred to $\mathbf{q}$ -space, and here the new integrand is proportional to $\hat{\mathbf{e}}_-(-\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_+(\hat{\mathbf{q}})$ (see (16.35)). To within an overall phase factor the vector product of the helicity unit-vectors equals $\hat{\mathbf{e}}_+(\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_+(\hat{\mathbf{q}}) = \mathbf{0}$. Altogether, it thus appears that $\mathbf{\Delta} = \mathbf{0}$, so that

$$\mathbf{P}_{\text{trans}} = \mathbf{P}. \quad (16.53)$$

Now it will be demonstrated that $\mathbf{P}$ is just the quantum mechanical mean value of the photon momentum operator $\mathbf{p} = \hbar \mathbf{q}$, the mean value being calculated in the momentum representation of wave mechanics. By means of the Parseval–Plancherel relation (9.56) one immediately obtains from (16.51)

$$\begin{aligned} \mathbf{P} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \left\{ \left[\mathbf{f}_+^{(+)}(\mathbf{q}, c_0 q) \right]^* \times \mathbf{f}_+^{(+)}(\mathbf{q}, c_0 q) - \left[\mathbf{f}_-^{(+)}(\mathbf{q}, c_0 q) \right]^* \right. \\ \left. \times \mathbf{f}_-^{(+)}(\mathbf{q}, c_0 q) \right\} \frac{d^3 q}{(2\pi)^3}, \end{aligned} \quad (16.54)$$

and thereafter with the help of (16.41)

$$\begin{aligned} \mathbf{P} = & \frac{1}{i c_0} \int_{-\infty}^{\infty} \left[\left| f_+^{(+)}(\mathbf{q}, c_0 q) \right|^2 \hat{\mathbf{e}}_+^*(\hat{\mathbf{q}}) \times \mathbf{e}_+(\hat{\mathbf{q}}) \right. \\ & \left. - \left| f_-^{(+)}(\mathbf{q}, c_0 q) \right|^2 \hat{\mathbf{e}}_-^*(\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_-(\hat{\mathbf{q}}) \right] \frac{d^3 q}{(2\pi)^3}. \end{aligned} \quad (16.55)$$

The vector products of the helicity unit vectors are simply

$$\hat{\mathbf{e}}_+^*(\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_+(\hat{\mathbf{q}}) = -\hat{\mathbf{e}}_-^*(\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_-(\hat{\mathbf{q}}) = i \hat{\mathbf{q}}, \quad (16.56)$$

as may readily be verified from (15.51), (15.53), and (15.54). The photon momentum hence is given by

$$\mathbf{P} = \frac{1}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \hbar \mathbf{q} \left| f_s^{(+)}(\mathbf{q}, c_0 q) \right|^2 \frac{d^3 q}{(2\pi)^3 q}, \quad (16.57)$$

and this expression has the same structure as (16.43) for the photon energy. By elimination of $f_{\pm}^{(+)}$ in favour of $g_{\pm}$ (16.44), and use of (16.45), the one-photon momentum appears as the quantum mechanical mean value of the momentum operator $\mathbf{p}$, i.e.,

$$\mathbf{P} = \sum_{s=+,-} \int_{-\infty}^{\infty} g_s^*(\mathbf{p}; t) \mathbf{p} g_s(\mathbf{p}; t) d^3 p. \quad (16.58)$$

On the basis of (16.46) and (16.58) it is realized that the contravariant one-photon energy–momentum four-vector (15.93) is the quantum mechanical mean value of the four-vector momentum operator that is

$$\{P^{\mu}\} = \int_{-\infty}^{\infty} \{p^{\mu}\} \left[\sum_{s=+,-} g_s^*(\mathbf{p}; t) \mathbf{p} g_s(\mathbf{p}; t) \right] d^3 p. \quad (16.59)$$

At this stage the reader should notice the analogy between the formulas for $\{P^{\mu}\}$ in the complex field theory (15.94) and the energy wave function formalism (16.59).

16.1.4 Lorentz-Invariant Integration on the Light Cone

Let us now consider the quantum mechanical mean value of the photon energy–momentum four-vector as this will appear in terms of the Riemann–Silberstein scalar amplitudes $f_{\pm}^{(+)}(\mathbf{q}, c_0 q)$. The explicit expression, which appears directly from (16.43) and (16.57), is

$$\{P^{\mu}\} = \frac{1}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \{p^{\mu}\} \left| f_s^{(+)}(\mathbf{q}, c_0 q) \right|^2 \frac{d^3 q}{(2\pi)^3 q}. \quad (16.60)$$

From a nonrelativistic point of view the quantity $(2\pi)^{-3}|f_s^{(+)}(\mathbf{q}, c_0q)|^2$ is not the energy probability density for photons of helicity s , because the standard quantum mechanical mean value of $\{p^\mu\}$ with such a distribution would not give us $\{P^\mu\}$. Only with the presence of the “extra” factor $(\hbar c_0q)^{-1}$ in the integrand one obtains $\{P^\mu\}$. If this extra factor is included in the probability density, one attains with $g_\pm(\mathbf{p})$ (16.44) the familiar quantum mechanical mean value form (16.59). However, since photon wave mechanics necessarily must be relativistic, it turns out, as I shall briefly indicate below, that the expression in (16.60) in fact has the correct mean value form. Before reaching this conclusion we discuss the problem in a slightly broader framework.

Let us consider a three-vector $\mathbf{H}(\mathbf{q}, q^0)$ which is a function of the components of the four-wave-vector $\{q^\mu\} = (q^0 = \omega/c_0, \mathbf{q})$. For a particle (or antiparticle) with rest mass m , the relativistic energy–momentum relation (7.61)

$$E^2 = (pc_0)^2 + (mc_0^2)^2 \quad (16.61)$$

is synonymous with the dispersion relation

$$(q^0)^2 = q^2 + Q_C^2, \quad (16.62)$$

where

$$Q_C = \frac{mc_0}{\hbar} \quad (16.63)$$

is the particle’s Compton wave number, as one finds by division of (16.61) with $(c_0\hbar)^2$. We now make a four-dimensional integration (volume element: $dq^0 d^3q/(2\pi)^4$) of $\mathbf{H}(\mathbf{q}, q^0)$ on the three-dimensional surface defined by the branch of the dispersion relation for which $q^0 > 0$. This operation gives us the Lorentz-invariant integral formula

$$\mathbf{I} = (2\pi)^{-4} \int_{-\infty}^{\infty} \theta(q^0) \delta[(q^0)^2 - q^2 - Q_C^2] \mathbf{H}(\mathbf{q}, q^0) dq^0 d^3q, \quad (16.64)$$

where $\theta(q^0)$ is the Heaviside step function. The condition $q^0 > 0$, which is ensured by $\theta(q^0)$, means that we are dealing with a particle, and not its antiparticle. Since

$$\begin{aligned} \theta(q^0) \delta[(q^0)^2 - q^2 - Q_C^2] &= \theta(q^0) \delta \left[(q^0 - \sqrt{q^2 + Q_C^2})(q^0 + \sqrt{q^2 + Q_C^2}) \right] \\ &= \frac{1}{2\sqrt{q^2 + Q_C^2}} \delta \left(q^0 - \sqrt{q^2 + Q_C^2} \right), \end{aligned} \quad (16.65)$$

the integral in (16.64) can be reduced to the simpler form

$$\mathbf{I} = \frac{1}{4\pi} \int_{-\infty}^{\infty} \mathbf{H}(\mathbf{q}, \sqrt{q^2 + Q_C^2}) \frac{d^3q}{(2\pi)^3 \sqrt{q^2 + Q_C^2}}. \quad (16.66)$$

For integration on the positive-frequency ($\omega = c_0 q^0 > 0$) branch of the particle dispersion relation the Lorentz-invariant volume element therefore is $d^3q/[(2\pi)^3 \sqrt{q^2 + Q_C^2}]$. For the massless photon the Compton wave number is zero, and consequently one has

$$I_{\text{photon}} = \frac{1}{4\pi} \int_{-\infty}^{\infty} H(\mathbf{q}, q) \frac{d^3q}{(2\pi)^3 q}. \quad (16.67)$$

The invariant volume element for integrations on the light cone hence is exactly the quantity $d^3q/[(2\pi)^3 q]$ appearing in (16.60). From this equation it finally follows that $|f_s^{(+)}(\mathbf{q}, c_0 q)|^2$ is a Lorentz-invariant function.

16.2 Relation Between the Energy Wave Function and Complex Field Formalisms in Direct Space

In Sect. 15.7, it was shown that the two primary vectorial photon wave functions of the complex field theory, i.e., $\beta_{\pm}^{(+)}(\mathbf{r}, t)$, were related in a spatially nonlocal (but timely local) manner to certain linear combinations of the analytical parts of the electric ($\mathbf{e}_T^{(+)}(\mathbf{r}, t)$) and magnetic ($\mathbf{b}^{(+)}(\mathbf{r}, t)$) field vectors, see (15.144). It appears from (16.23) that these combinations are precisely the ones which define the vectorial energy wave functions $f_{\pm}^{(+)}(\mathbf{r}, t)$, see (16.23). With the kernel $k(|\mathbf{r} - \mathbf{r}'|)$ in (15.145) given by the regularized expression in (15.148), one obtains the following identical nonlocal relations between $\beta_{\pm}^{(+)}(\mathbf{r}, t)$ and $f_{\pm}^{(+)}(\mathbf{r}, t)$:

$$\beta_{\pm}^{(+)}(\mathbf{r}, t) = \frac{\sqrt{2}}{4} (2\pi)^{-3} \frac{1}{\sqrt{\hbar c_0}} \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-5/2} f_{\pm}^{(+)}(\mathbf{r}', t) d^3 r'. \quad (16.68)$$

In the complex field theory, the normalization condition on the spinorial photon wave function $\Phi^{\text{CF}}(\mathbf{r}, t)$ is given by a single spatial integral (15.116). With the help of (15.114) the normalization condition can be expressed in terms of the $\beta_{\pm}^{(+)}(\mathbf{r}, t)$'s. Thus,

$$(2\pi)^3 \sum_{s=+,-} \int_{-\infty}^{\infty} [\beta_s^{(+)}(\mathbf{r}, t)]^* \cdot \beta_s^{(+)}(\mathbf{r}, t) d^3 r = 1. \quad (16.69)$$

Let us now see which form this normalization condition takes when expressed in terms of the energy wave functions $f_{\pm}^{(+)}(\mathbf{r}, t)$. By inserting the expression in (16.68) into (16.69) and inverting the order of integrations one obtains

$$\frac{(2\pi)^{-3}}{8\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} I(\mathbf{r}' - \mathbf{r}'') [\mathbf{f}_s^{(+)}(\mathbf{r}', t)]^* \cdot \mathbf{f}_s^{(+)}(\mathbf{r}'', t) d^3 r'' d^3 r' = 1, \quad (16.70)$$

where

$$I(\mathbf{r}' - \mathbf{r}'') = \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-5/2} |\mathbf{r} - \mathbf{r}''|^{-5/2} d^3 r. \quad (16.71)$$

The integral in (16.71) may easily be determined with the help of the regularized integral expression

$$R^{-5/2} = 2(2\pi)^{-3/2} \int_{-\infty}^{\infty} q^{-1/2} e^{i\mathbf{q} \cdot \mathbf{R}} d^3 q. \quad (16.72)$$

A comparison of (15.145) and (15.148) immediately shows the correctness of (16.72). Hence,

$$I(\mathbf{r}' - \mathbf{r}'') = 4(2\pi)^{-3} \int_{-\infty}^{\infty} q^{-1/2} Q^{-1/2} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{i\mathbf{Q} \cdot (\mathbf{r} - \mathbf{r}'')} d^3 r d^3 Q d^3 q, \quad (16.73)$$

and thereafter we obtain, via

$$\int_{-\infty}^{\infty} e^{i(\mathbf{q} + \mathbf{Q}) \cdot \mathbf{r}} d^3 r = (2\pi)^3 \delta(\mathbf{q} + \mathbf{Q}), \quad (16.74)$$

the simple expression

$$I(\mathbf{r}' - \mathbf{r}'') = 4 \int_{-\infty}^{\infty} q^{-1} e^{i\mathbf{q} \cdot (\mathbf{r}'' - \mathbf{r}')} d^3 q. \quad (16.75)$$

Integration in spherical coordinates (polar axis along the direction of $\mathbf{r}'' - \mathbf{r}'$) and a *regularization* of the radial integration at infinity give

$$I(\mathbf{r}' - \mathbf{r}'') = \frac{16\pi}{|\mathbf{r}' - \mathbf{r}''|^2}. \quad (16.76)$$

With this for $I(\mathbf{r}' - \mathbf{r}'')$, (16.70) is reduced to the form

$$\frac{(2\pi)^{-2}}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} |\mathbf{r}' - \mathbf{r}''|^{-2} \left[\mathbf{f}_s^{(+)}(\mathbf{r}', t) \right]^* \cdot \mathbf{f}_s^{(+)}(\mathbf{r}'', t) d^3 r'' d^3 r' = 1, \quad (16.77)$$

which in spinor notation (16.26) can be written as follows:

$$\frac{(2\pi)^{-2}}{\hbar c_0} \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-2} \Phi^+(\mathbf{r}, t) \cdot \Phi(\mathbf{r}', t) d^3 r' d^3 r = 1. \quad (16.78)$$

The presence of the scaling factor $(c_0 p)^{-1/2}$ in (16.44) has the consequence that the one-photon normalization condition, which in momentum space is given by a single (three-dimensional) integral (16.48), in direct space is given by a double integral. The strength of the “correlation” between different spatial parts of the wave function $\Phi(\mathbf{r}, t)$ is given by the function $|\mathbf{r} - \mathbf{r}'|^{-2}$.

16.3 Wave Mechanics of Longitudinal and Scalar Photons: Standard Theory

The photon is concept of free space, but observational effects are always related to photon–matter interactions. In such interactions photons are either destroyed or created. In free space, there is no unique photon wave function. Various constructions with justice can be considered as representatives for a free photon. In the framework of semiclassical electrodynamics, the only thing which matter, in a sense, is that the interaction described in terms of the classical Maxwell–Lorentz equations and the Schrödinger (or Pauli, Dirac, Klein–Gordon) equation takes the correct form. In this and the previous chapter two important constructions have been discussed: (1) The complex field theory and (2) the energy wave function formalism. From a relativistic point of view it is often important to work with a manifestly covariant theory, and such a formalism requires the introduction of two new types of photons in free space. In the new formulation the potential four-vector and the Lorenz gauge play essential roles. In the remaining part of this chapter I shall briefly discuss two slightly different yet physically equivalent approaches to manifestly covariant photon wave mechanics. Exemplified by the approach discussed in Sect. 16.4, I shall argue that the covariant description not only is of interest in the relativistic domain but that it also may serve as a springboard for introduction of a new near-field photon concept. As we shall realize later on in this book, near-field photon wave mechanics allows us to see electrodynamic near-field interactions in a new perspective, and it furthermore enables us to address near-field quantum optical problems in a novel manner.

16.3.1 Complex Field Theory in Terms of the Transverse Vector Potential

The starting point for the present introduction of longitudinal and scalar photon wave functions is the complex field formalism discussed in Chap. 15. In the momentum (wave vector)–time domain two positive-frequency complex field vectors, $\beta_{\pm}^{(+)}(\mathbf{q}; t)$, were introduced by the definitions in (15.65), and in the photon spinor description these vectors enter the upper- and lower-parts of the photon wave function, see (15.74). For what follows it is convenient to emphasize that the $\beta_{\pm}^{(+)}$'s appear in the formalism for transverse photons. We do this by adding a subscript T, i.e.,

$$\beta_{T,\pm}^{(+)}(\mathbf{q}; t) \equiv \beta_{\pm}^{(+)}(\mathbf{q}; t). \quad (16.79)$$

In the expression for the complex field, the electric and magnetic field vectors are replaced by the analytical part of the transverse vector potential, $\mathbf{a}_T^{(+)}(\mathbf{q}; t)$ (a small letter is used for the vector- and scalar potentials here and below to indicate that these are related to the one-photon formalism). Since (9.39) and (9.40) take the

forms

$$\mathbf{B}(\mathbf{q}; t) = i\mathbf{q} \times \mathbf{A}_T(\mathbf{q}; t), \quad (16.80)$$

$$E_T(\mathbf{q}; t) = -\frac{\partial}{\partial t} A_T(\mathbf{q}; t) \quad (16.81)$$

in the $(\mathbf{q}; t)$ -domain, one has

$$\mathbf{b}^{(+)}(\mathbf{q}; t) = i\mathbf{q} \times \mathbf{a}_T^{(+)}(\mathbf{q}; t), \quad (16.82)$$

$$e_T^{(+)}(\mathbf{q}; t) = -\frac{\partial}{\partial t} a_T^{(+)}(\mathbf{q}; t), \quad (16.83)$$

and consequently from (15.65)

$$\beta_{T,\pm}^{(+)}(\mathbf{q}; t) = \frac{(2\pi)^{-3/2}}{N_\beta(q)} \left(-\frac{\partial}{\partial t} a_T^{(+)}(\mathbf{q}; t) \mp c_0 q \hat{\mathbf{q}} \times \mathbf{a}_T^{(+)}(\mathbf{q}; t) \right). \quad (16.84)$$

The amplitudes of the $\beta_\pm^{(+)}$'s, given by (15.78), can be related to the helicity components of $\mathbf{a}_T^{(+)}$, i.e.,

$$a_{T,\pm}^{(+)}(\mathbf{q}; t) = \hat{\mathbf{e}}_\pm^*(\hat{\mathbf{q}}) \cdot \mathbf{a}_T^{(+)}(\mathbf{q}; t) \quad (16.85)$$

by scalar multiplication of (16.84) with $\hat{\mathbf{e}}_\pm^*(\hat{\mathbf{q}})$. Since, with the help of the complex conjugates of (15.72), one obtains

$$\begin{aligned} \hat{\mathbf{e}}_\pm^* \cdot \hat{\mathbf{q}} \times \mathbf{a}_T^{(+)} &= -\hat{\mathbf{q}} \times \hat{\mathbf{e}}_\pm^* \cdot \mathbf{a}_T^{(+)} = \mp i \hat{\mathbf{e}}_\pm^* \cdot \mathbf{a}_T^{(+)} \\ &= \mp i a_{T,\pm}^{(+)}, \end{aligned} \quad (16.86)$$

it appears that

$$\beta_{T,\pm}^{(+)}(\mathbf{q}; t) = \frac{i(2\pi)^{-3/2}}{N_\beta(q)} \left(c_0 q + i \frac{\partial}{\partial t} \right) a_{T,\pm}^{(+)}(\mathbf{q}; t). \quad (16.87)$$

The gauge invariance of the $a_{T,\pm}^{(+)}$'s implies that the $\beta_{T,\pm}^{(+)}$'s are gauge invariant, as we already knew. The wave functions for the two transverse photons obey the Schrödinger-like wave equations in (15.73).

16.3.2 Longitudinal and Scalar Photon Wave Functions, and Their Related Wave Equations

A photon wave function related to the longitudinal part of the electric field cannot be introduced in analogy to what was done in (15.65) since the longitudinal electric

field is not “accompanied” by a longitudinal magnetic field, and the Maxwell–Lorentz equations do not allow the establishment of a dynamical wave equation (Schrödinger equation) for the longitudinal field amplitude. With the reformulation given in (16.87) a natural choice for a longitudinal photon wave function in the momentum–time domain, $\beta_L^{(+)}(\mathbf{q}; t)$, emerges by simply replacing $a_{T,\pm}^{(+)}$ with the analytical part, $a_L^{(+)} = \hat{\mathbf{q}} \cdot \mathbf{a}_L^{(+)}$, of the longitudinal vector potential. Hence, one defines the (scalar) wave function of a longitudinal photon by

$$\beta_L^{(+)}(\mathbf{q}; t) = \frac{i(2\pi)^{-3/2}}{N_\beta(q)} \left(c_0 q + i \frac{\partial}{\partial t} \right) a_L^{(+)}(\mathbf{q}; t). \quad (16.88)$$

In order for this construction to be meaningful, we *require* that the wave function satisfies a dynamical equation analogous in form to the one given in (15.73), viz.,

$$i\hbar \frac{\partial}{\partial t} \beta_L^{(+)}(\mathbf{q}; t) = c_0 \hbar q \beta_L^{(+)}(\mathbf{q}; t). \quad (16.89)$$

The requirement necessitates that $a_L^{(+)}$ must obey the differential equation

$$(c_0 q - i \frac{\partial}{\partial t})(c_0 q + i \frac{\partial}{\partial t}) a_L^{(+)}(\mathbf{q}; t) = 0, \quad (16.90)$$

as one realizes by inserting (16.88) into (16.89). We know that the longitudinal part of the vector potential is gauge dependent, and it appears from the analysis in Sect. 9.2.4 that $\mathbf{A}_L(\mathbf{r}, t)$ in the Lorenz gauge satisfies the wave equation $\square \mathbf{A}_L(\mathbf{r}, t) = \mathbf{0}$ in free space; see (9.48). In the $\mathbf{q}$ -domain the analytical part of $\mathbf{A}_L$, therefore satisfies the equation

$$\left[(c_0 q)^2 + \frac{\partial^2}{\partial t^2} \right] \mathbf{A}_L^{(+)}(\mathbf{q}; t) = \mathbf{0}. \quad (16.91)$$

With the replacement $\mathbf{A}_L^{(+)} \Rightarrow a_L^{(+)}$, (16.91) leads to the equation

$$\left[(c_0 q)^2 + \frac{\partial^2}{\partial t^2} \right] a_L^{(+)}(\mathbf{q}; t) = 0 \quad (16.92)$$

for the amplitude, $a_L^{(+)}(\mathbf{q}; t)$. The identity of (16.90) and (16.92), thus has brought us to the conclusion that the wave function of the longitudinal photon (16.88) satisfies the Schrödinger-like equation in (16.89) *provided* the longitudinal part of the vector potential refers to the Lorenz gauge.

The potential description of electromagnetics in free space also involves a scalar potential, A_0 . From the point of view of photon wave mechanics it is thus obvious that a scalar photon wave function, $\beta_0^{(+)}(\mathbf{q}; t)$, should be introduced via the definition

$$\beta_0^{(+)}(\mathbf{q}; t) = \frac{i(2\pi)^{-3/2}}{N_\beta(q)} \left(c_0 q + i \frac{\partial}{\partial t} \right) a_0^{(+)}(\mathbf{q}; t). \quad (16.93)$$

In analogy with what was done in the case of the longitudinal photon one *requires* that the wave function of the scalar photon satisfies the dynamical equation

$$i\hbar \frac{\partial}{\partial t} \beta_0^{(+)}(\mathbf{q}; t) = c_0 \hbar q \beta_0^{(+)}(\mathbf{q}; t). \quad (16.94)$$

In order for this to be correct the analytical part of the scalar potential must obey the differential equation

$$(c_0 q - i \frac{\partial}{\partial t})(c_0 q + i \frac{\partial}{\partial t}) a_0^{(+)}(\mathbf{q}; t) = 0. \quad (16.95)$$

Above, it was found that one must work in the Lorenz gauge in order to introduce a longitudinal photon concept in analogy to the transverse photon concept. For consistency, the scalar potential thus must be the one associated to the Lorenz gauge. In this gauge, the free-space scalar potential $A_0(\mathbf{r}, t)$ satisfies the wave equation $\square A_0(\mathbf{r}, t) = 0$; see (2.15) with $\phi(\mathbf{r}, t)$ replaced by $c_0 A_0(\mathbf{r}, t)$. In turn, it is obvious in view of the discussion for the longitudinal dynamics that $a_0^{(+)}(\mathbf{q}; t)$ obeys the equation

$$\left[(c_0 q)^2 + \frac{\partial^2}{\partial t^2} \right] a_0^{(+)}(\mathbf{q}; t) = 0, \quad (16.96)$$

which is the nothing more than (16.95). In conclusion we have thus realized that in the Lorenz gauge longitudinal and scalar photons can be introduced in a manner which makes a natural bridge to the transverse photon concept.

As it was the case in the complex field theory, the presence of the q -dependent normalization factor $N_\beta(q)$ in itself results in a spatially nonlocal relation between the longitudinal and scalar photon wave functions and the electromagnetic potentials in direct space. Also, the $c_0 q$ -term in the parentheses on the right side of (16.88) and (16.94) contributes to the spatial nonlocality between the wave function and the potential.

16.3.3 Identity of the Longitudinal and Scalar Photons

In free space, the longitudinal part of the electric field is zero everywhere in space to all times, and the electromagnetic net effect of the longitudinal and scalar photons must therefore vanish in all space–time points. In the presence of matter, the electrodynamic effects of these photons do not extinguish each other, except in the far field of the particle system. Seen in this perspective the longitudinal and scalar photons only play a physical role in field–matter interactions, and, as we shall realize, only at times where the interaction is present. No free propagation effects emerge from

the presence of longitudinal and scalar photons. It is therefore these photon types often are classified as virtual photons.

Let us now prove that the wave functions of the longitudinal and scalar photons are identical in free space. From the Lorenz gauge condition (9.47) between the longitudinal vector potential, $A_L(\mathbf{r}, t)$, and the scalar potential, $A_0(\mathbf{r}, t) = \phi(\mathbf{r}, t)/c_0$, follows the constraint

$$iqc_0 a_L^{(+)}(\mathbf{q}; t) + \frac{\partial}{\partial t} a_0^{(+)}(\mathbf{q}; t) = 0 \quad (16.97)$$

between the photon potentials in the wave-vector representation. As an immediate consequence of (9.41), it appears that the analytical part of the longitudinal electric field is given by

$$\mathbf{e}_L^{(+)}(\mathbf{q}; t) = -\frac{\partial}{\partial t} \mathbf{a}_L^{(+)}(\mathbf{q}; t) - ic_0 \mathbf{q} a_0^{(+)}(\mathbf{q}; t) \quad (16.98)$$

in the $\mathbf{q}$ -domain. To emphasize that our discussion relates to the photons the longitudinal electric field is denoted by a small letter. In free space $\mathbf{e}_L^{(+)}(\mathbf{q}; t) = \mathbf{0}$, and in this case the photon amplitudes are related by the equation

$$\frac{\partial}{\partial t} a_L^{(+)}(\mathbf{q}; t) + ic_0 a_0^{(+)}(\mathbf{q}; t) = 0. \quad (16.99)$$

By addition of (16.97) and (16.99) one obtains

$$\left(c_0 q + i \frac{\partial}{\partial t}\right) a_L^{(+)}(\mathbf{q}, t) = \left(c_0 q + i \frac{\partial}{\partial t}\right) a_0^{(+)}(\mathbf{q}; t), \quad (16.100)$$

and a comparison of this equation to (16.88) and (16.93) immediately leads to the conclusion

$$\beta_L^{(+)}(\mathbf{q}; t) = \beta_0^{(+)}(\mathbf{q}; t), \quad (16.101)$$

i.e., the identity of the longitudinal and scalar photon wave functions in free space.

16.3.4 Quantum Mechanical Mean Values of the Longitudinal and Scalar Photon Energies

Let us temporarily assume that the longitudinal electric field does not vanish. By addition of (16.97) and the scalar product of (16.98) with $\hat{\mathbf{q}}$ one obtains with $e_L^{(+)}(\mathbf{q}; t) = \hat{\mathbf{q}} \cdot \mathbf{e}_L^{(+)}(\mathbf{q}, t)$

$$e_L^{(+)}(\mathbf{q}; t) = i \left(c_0 q + i \frac{\partial}{\partial t} \right) \left[a_L^{(+)}(\mathbf{q}; t) - a_0^{(+)}(\mathbf{q}; t) \right], \quad (16.102)$$

and then, with the help of (16.88) and (16.93),

$$e_L^{(+)}(\mathbf{q}; t) = (2\pi)^{3/2} N_\beta(q) \left[\beta_L^{(+)}(\mathbf{q}; t) - \beta_0^{(+)}(\mathbf{q}; t) \right]. \quad (16.103)$$

In $\mathbf{q}$ -space the energy density associated to $e_L^{(+)}(\mathbf{q}; t)$ is proportional to

$$\begin{aligned} & (2\pi)^{-3} \left(e_L^{(+)}(\mathbf{q}; t) \right)^* e_L^{(+)}(\mathbf{q}; t) \\ &= N_\beta^2(q) \left\{ \left| \beta_L^{(+)} \right|^2 + \left| \beta_0^{(+)} \right|^2 - \left[\beta_0^{(+)} \left(\beta_L^{(+)} \right)^* + c.c. \right] \right\}, \end{aligned} \quad (16.104)$$

In free space, where $e_L^{(+)}(\mathbf{q}; t) = 0$, one obtains utilizing (15.66), and (16.101) in the mixed terms, $\beta_0^{(+)}(\beta_L^{(+)})^* + c.c.$, the following expression:

$$\int_{-\infty}^{\infty} \hbar c_0 q \left(\left| \beta_L^{(+)}(\mathbf{q}; t) \right|^2 - \left| \beta_0^{(+)}(\mathbf{q}; t) \right|^2 \right) d^3 q = 0. \quad (16.105)$$

One may assert that the term containing $|\beta_L^{(+)}|^2$ in (16.105) represent the quantum mechanical mean value of the field energy attached to the longitudinal photon. The minus sign in front of $|\beta_0^{(+)}|^2$ indicates that the mean energy of the scalar photon is negative. In a sense one may claim that a plane-wave scalar photon has a *negative* energy $-\hbar c_0 q$. It is thus the association of a negative energy to the scalar photon which leads to a vanishing of the sum of the field energies of the longitudinal and scalar photons everywhere in space.

16.4 Wave Mechanics of Gauge and Near-Field Photons

When electromagnetic fields interact with matter the longitudinal and scalar photon variables no longer extinguish each other in the rim zone. In near-field electrodynamics the maintenance of manifest covariance is seldom so important. The longitudinal electric field is always of crucial importance, however. Since this field in photon wave mechanics involves the difference between the wave functions of the longitudinal and scalar photons (see (16.103)), is convenient to introduce two new photon types by linear combination of the original ones. In this manner, a new so-called near-field photon is introduced. The new photon variable relates in a direct way to the longitudinal electric field in the rim zone. It is quite possible to introduce a near-field photon starting from the formalism developed in Sect. 16.3. Below I

shall do it using a slightly different approach, however. In the same manner, as the photon energy wave function formalism evolved from the complex field theory by omission of the q -dependent normalization factor $N_\beta(q)$ (15.66), we now introduce longitudinal and scalar photons in the space–time domain directly on the basis of the analytical parts of the longitudinal and scalar potentials.

16.4.1 Transverse Photon Schrödinger-Like Equations in Direct and Reciprocal Space

In free space, the analytical part of the transverse vector potential, $A_T^{(+)}(\mathbf{r}, t)$, satisfies the wave equation

$$\square A_T^{(+)}(\mathbf{r}, t) = 0. \quad (16.106)$$

After a proper normalization one arrives at the vectorial one-photon potential $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$. Later on we shall discuss how one may normalize photon wave functions by means of the emission process from the photon source. Now, we formally factorize the d’Lambertian operator as follows:

$$-\square = \left(\sqrt{-\nabla^2} + \frac{i}{c_0} \frac{\partial}{\partial t} \right) \left(\sqrt{-\nabla^2} - \frac{i}{c_0} \frac{\partial}{\partial t} \right), \quad (16.107)$$

where the definition of the nonlocal operator $i\sqrt{-\nabla^2} = \sqrt{\Delta}$ appears from (15.21). It is obvious that all solutions to the integro-differential equation

$$i\hbar \frac{\partial}{\partial t} \mathbf{a}_T^{(+)}(\mathbf{r}, t) = c_0\hbar \sqrt{-\nabla^2} \mathbf{a}_T^{(+)}(\mathbf{r}, t) \quad (16.108)$$

are solutions also to (16.106) (with $A_T^{(+)} = \mathbf{a}_T^{(+)}$). One may consider (16.108) as the quantum mechanical wave equation for a transverse vectorial photon wave function $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$. In reciprocal space (16.108) takes the form

$$i\hbar \frac{\partial}{\partial t} \mathbf{a}_T^{(+)}(\mathbf{q}; t) = c_0\hbar q \mathbf{a}_T^{(+)}(\mathbf{q}; t), \quad (16.109)$$

where $c_0\hbar q$ is the Hamilton operator in $\mathbf{q}$ -space. The Hamilton operator in direct space, i.e., $\mathcal{H}(R) = c_0\hbar \sqrt{-\nabla^2}$, is as we know from the analysis in Sect. 15.5.2 a spatially nonlocal and singular operator; see (15.118) and (15.124). Two transverse scalar photon wave functions can of course be defined by expanding $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$ after two orthogonal (and in general complex) unit vectors lying in a plane perpendicular to $\mathbf{q}$.

16.4.2 Longitudinal and Scalar Photons Once More

In the Lorenz gauge, the analytical parts of the longitudinal [$a_L^{(+)}(\mathbf{r}, t)$] and scalar [$a_0^{(+)}(\mathbf{r}, t)$] potentials satisfy in free space identical wave equations, viz.,

$$\square a_L^{(+)}(\mathbf{r}, t) = 0, \quad (16.110)$$

$$\square a_0^{(+)}(\mathbf{r}, t) = 0. \quad (16.111)$$

To emphasize that we are aiming at a description of single photons small letters are again used to denote the relevant potentials. By following the same line of reasoning as was used in Sect. 16.4.1 we can establish dynamical equations

$$i\hbar \frac{\partial}{\partial t} a_L^{(+)}(\mathbf{r}, t) = c_0 \hbar \sqrt{-\nabla^2} a_L^{(+)}(\mathbf{r}, t), \quad (16.112)$$

and

$$i\hbar \frac{\partial}{\partial t} a_0^{(+)}(\mathbf{r}, t) = c_0 \hbar \sqrt{-\nabla^2} a_0^{(+)}(\mathbf{r}, t) \quad (16.113)$$

for the potentials. The longitudinal [$a_L^{(+)}(\mathbf{r}, t)$] and scalar [$a_0^{(+)}(\mathbf{r}, t)$] potentials we now consider as longitudinal (vectorial) and scalar photon wave functions, and (16.112) and (16.113) are the Schrödinger-like quantum mechanical wave equations they satisfy. In the wave-vector–time domain the dynamical equations take the forms

$$i\hbar \frac{\partial}{\partial t} a_L^{(+)}(\mathbf{q}; t) = c_0 \hbar q a_L^{(+)}(\mathbf{q}; t), \quad (16.114)$$

$$i\hbar \frac{\partial}{\partial t} a_0^{(+)}(\mathbf{q}; t) = c_0 \hbar q a_0^{(+)}(\mathbf{q}; t). \quad (16.115)$$

In the case of the longitudinal photon, use has been made of the fact that the potential can be decomposed as

$$a_L^{(+)}(\mathbf{q}; t) = a_L^{(+)}(\mathbf{q}; t) \hat{\mathbf{q}}, \quad (16.116)$$

and the Schrödinger-like equation in (16.114) is for the amplitude, $a_L^{(+)}(\mathbf{q}; t)$, of the longitudinal potential.

In free space, the wave functions of the longitudinal and scalar photons are identical since the analytical part of the longitudinal electric field is identically zero, i.e.,

$$\mathbf{e}_L^{(+)}(\mathbf{q}; t) = 0. \quad (16.117)$$

The proof for this claim follows readily if one first multiplies (16.114) by $\hat{\mathbf{q}}$, and thereafter inserts the resulting expression for the time derivative of $a_L^{(+)}(\mathbf{q}; t)$, namely

$$\frac{\partial}{\partial t} a_L^{(+)}(\mathbf{q}; t) = -i c_0 q a_L^{(+)}(\mathbf{q}; t), \quad (16.118)$$

into (16.98). Thus, it appears that

$$\mathbf{e}_L^{(+)}(\mathbf{q}; t) = i c_0 \mathbf{q} \left(a_L^{(+)}(\mathbf{q}; t) - a_0^{(+)}(\mathbf{q}; t) \right) \quad (16.119)$$

and together (16.117) and (16.119) show that

$$a_L^{(+)}(\mathbf{q}; t) = a_0^{(+)}(\mathbf{q}; t), \quad (16.120)$$

as claimed above. The result in (16.120) also follows immediately by insertion of (16.114) into (16.99).

16.4.3 Gauge and Near-Field Photons

Let us temporarily forget that the longitudinal and scalar photon wave functions are identical in free space. In $\mathbf{q}$ -space, two new photons, named the gauge (G) and near-field (NF) photon, with related analytical potentials $a_G^{(+)}(\mathbf{q}; t)$ and $a_{NF}^{(+)}(\mathbf{q}; t)$, respectively, are now introduced via the unitary transformation

$$\mathbf{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} \quad (16.121)$$

as follows

$$\begin{pmatrix} a_{NF}^{(+)}(\mathbf{q}; t) \\ a_G^{(+)}(\mathbf{q}; t) \end{pmatrix} = \mathbf{T} \begin{pmatrix} a_L^{(+)}(\mathbf{q}; t) \\ a_0^{(+)}(\mathbf{q}; t) \end{pmatrix}. \quad (16.122)$$

The reason that the new photons have been named the gauge and near-field photon will appear shortly. In explicit form, the transformation in (16.122) is given by

$$a_{NF}^{(+)}(\mathbf{q}; t) = \frac{i}{\sqrt{2}} \left(a_L^{(+)}(\mathbf{q}; t) - a_0^{(+)}(\mathbf{q}; t) \right), \quad (16.123)$$

$$a_G^{(+)}(\mathbf{q}; t) = \frac{1}{\sqrt{2}} \left(a_L^{(+)}(\mathbf{q}; t) + a_0^{(+)}(\mathbf{q}; t) \right). \quad (16.124)$$

By taking the time derivatives of (16.123) and (16.124) and utilizing (16.114) and (16.115) the reader may easily convince herself that the near-field and gauge wave functions satisfy the dynamical equations

$$i\hbar \frac{\partial}{\partial t} a_{NF}^{(+)}(\mathbf{q}; t) = c_0 \hbar q a_{NF}^{(+)}(\mathbf{q}; t), \quad (16.125)$$

$$i\hbar \frac{\partial}{\partial t} a_G^{(+)}(\mathbf{q}; t) = c_0 \hbar q a_G^{(+)}(\mathbf{q}; t). \quad (16.126)$$

In reciprocal space, these are the quantum mechanical wave equations for the new photon types. Although the near-field photon wave function formally satisfies the wave equation in (16.125), it appears from (16.120) and (16.123) that $a_{\text{NF}}^{(+)}(\mathbf{q}; t) = 0$ in free space. In the absence of field–matter interactions the near-field photon thus does not exist. The reason for this stems from the fact that

$$0 = e_L^{(+)}(\mathbf{q}; t) = \sqrt{2}c_0 \mathbf{q} a_{\text{NF}}^{(+)}(\mathbf{q}; t), \quad (16.127)$$

as one realizes by combining (16.119) and (16.123). The vanishing of the longitudinal electric field in free space thus implies the nonexistence of near-field photons. The simple connection between the longitudinal electric field and the near-field photon dynamical variable $a_{\text{NF}}^{(+)}(\mathbf{q}; t)$ indicates a potential usefulness of the near-field photon concept for rim-zone electrodynamics at both the first- and second-quantized level.

16.4.4 Gauge Transformations Within the Lorenz Gauge

We have realized previously that the microscopic electric and magnetic fields, expressed in terms of the vector and scalar potentials, are invariant against certain so-called gauge transformations of the potentials. In a gauge transformation, only the longitudinal part of the vector potential and the scalar potential change. In the space–time domain, a gauge function $\chi(\mathbf{r}, t)$ transforms these potentials as indicated in (2.12) and (9.43). In the potential theory of photon wave mechanics the covariant Lorenz gauge plays a central role, as we have seen. In this gauge the longitudinal vector potential and the scalar potential are linked via the constraint given in (9.47). The potentials are not completely fixed by the Lorenz gauge condition in (9.47), however. Thus, if one assumes that the potentials $A_L(\mathbf{r}, t)$ and $A_0(\mathbf{r}, t) [= c_0^{-1}\phi(\mathbf{r}, t)]$ satisfy the Lorenz condition in (9.47), is it then possible that new (superscript NEW) potentials, determined by the gauge transformation

$$A_L^{\text{NEW}}(\mathbf{r}, t) = A_L(\mathbf{r}, t) + \nabla f(\mathbf{r}, t), \quad (16.128)$$

$$A_0^{\text{NEW}}(\mathbf{r}, t) = A_0(\mathbf{r}, t) - \frac{1}{c_0} \frac{\partial}{\partial t} f(\mathbf{r}, t), \quad (16.129)$$

also can satisfy the Lorenz gauge condition? By inserting the expressions for A_L and A_0 obtained from (16.128) and (16.129) into (9.47) it is easy to show that the new potentials satisfy the Lorenz gauge condition

$$\nabla \cdot A_L^{\text{NEW}}(\mathbf{r}, t) + \frac{1}{c_0} \frac{\partial}{\partial t} A_0^{\text{NEW}}(\mathbf{r}, t) = 0, \quad (16.130)$$

provided the gauge function $f(\mathbf{r}, t)$ is a solution of the wave equation

$$\square f(\mathbf{r}, t) = 0. \quad (16.131)$$

16.4.5 Elimination of the Gauge Photon

In preparation, for use in the potential theory of photon wave mechanics, the following four modifications are now made in (16.128)–(16.131): (1) Transformation to the wave-vector–time domain, thereafter (2) a translation to analytical signals, then (3) an adjustment of the general analytical potentials to the one-photon values (small letters instead of capital letters), and finally (4) use of only the amplitude $A_L(\mathbf{q}; t)$ of the longitudinal vector potential, $\mathbf{A}_L(\mathbf{q}; t) = A_L(\mathbf{q}; t)\hat{\mathbf{q}}$. With these modifications the gauge transformation reads

$$a_L^{(+)\text{NEW}}(\mathbf{q}; t) = a_L^{(+)}(\mathbf{q}; t) + i q f^{(+)}(\mathbf{q}; t), \quad (16.132)$$

$$a_0^{(+)\text{NEW}}(\mathbf{q}; t) = a_0^{(+)}(\mathbf{q}; t) - \frac{1}{c_0} \frac{\partial}{\partial t} f^{(+)}(\mathbf{q}; t). \quad (16.133)$$

The constraint on the gauge function $f^{(+)}(\mathbf{q}; t)$ is given by the second-order differential equation

$$\left[(c_0 q)^2 + \frac{\partial^2}{\partial t^2} \right] f^{(+)}(\mathbf{q}; t) = 0. \quad (16.134)$$

Since $f^{(+)}(\mathbf{q}; t)$ is an analytical signal the constraint in (16.134) can be simplified to a first-order differential equation. To prove this we first transfer (16.134) to the frequency domain [$\partial/\partial t \rightarrow -i\omega$]. Here, it takes the form

$$(c_0 q + \omega)(c_0 q - \omega) f^{(+)}(\mathbf{q}, \omega) = 0, \quad (16.135)$$

but, since $f^{(+)}(\mathbf{q}, \omega) = 0$ for $\omega < 0$, the factor $c_0 q + \omega$ is nonvanishing (positive) for all relevant ω . The condition in (16.135) hence is identical to the condition

$$(c_0 q - \omega) f^{(+)}(\mathbf{q}, \omega) = 0. \quad (16.136)$$

When this equation is taken back to the time domain it follows that the constraint in (16.134) is tantamount to the requirement

$$(c_0 q - i \frac{\partial}{\partial t}) f^{(+)}(\mathbf{q}; t) = 0 \quad (16.137)$$

on the analytical gauge function. The Lorenz gauge condition among the photon wave functions already was given in (16.97).

Let us now investigate the consequences of the transformation analysis given above for the near-field and gauge photons. By inversion of the transformation given in (16.123) and (16.124), the reader may show that the Lorenz gauge condition in (16.97) corresponds to the constraint

$$(c_0 q - i \frac{\partial}{\partial t}) a_G^{(+)}(\mathbf{q}; t) = i(c_0 q + i \frac{\partial}{\partial t}) a_{NF}^{(+)}(\mathbf{q}; t) \quad (16.138)$$

between the wave functions of the gauge and near-field photon. How does the wave functions $a_{NF}^{(+)}(\mathbf{q}; t)$ and $a_G^{(+)}(\mathbf{q}; t)$ change when subjected to a gauge transformation within the Lorenz gauge? This question is answered by writing down the transformation in (16.122) among the new potentials $a_{NF}^{(+)\text{NEW}}$, $a_G^{(+)\text{NEW}}$, $a_L^{(+)\text{NEW}}$ and $a_0^{(+)\text{NEW}}$, and utilizing thereafter the gauge transformation in (16.132) and (16.133). Altogether, this results in the following relations between the original and new NF- and G-photon variables

$$a_{NF}^{(+)\text{NEW}}(\mathbf{q}; t) = a_{NF}^{(+)}(\mathbf{q}; t) - \frac{1}{c_0 \sqrt{2}} (c_0 q - i \frac{\partial}{\partial t}) f^{(+)}(\mathbf{q}; t), \quad (16.139)$$

$$a_G^{(+)\text{NEW}}(\mathbf{q}; t) = a_G^{(+)}(\mathbf{q}; t) + \frac{i}{c_0 \sqrt{2}} (c_0 q + i \frac{\partial}{\partial t}) f^{(+)}(\mathbf{q}; t). \quad (16.140)$$

To ensure that the new near-field and gauge photon wave functions remain within the Lorenz gauge, (16.137) must be obeyed. This immediately shows that the near-field photon wave function is invariant against transformations within the Lorenz gauge, i.e.,

$$a_{NF}^{(+)\text{NEW}}(\mathbf{q}; t) = a_{NF}^{(+)}(\mathbf{q}; t). \quad (16.141)$$

In a sense, the result in (16.141) is obvious due to the fact that the longitudinal electric field and thus also the near-field photon wave function vanish in free space; see (16.127). Even though the analytical part of the longitudinal electric field vanishes one cannot conclude that gauge photons cannot exist in free space, a priori. It is possible, however, to eliminate the gauge photon by a suitable gauge transformation within the Lorenz gauge. Thus, let us choose a gauge function

$$f^{(+)}(\mathbf{q}; t) = \frac{i}{q \sqrt{2}} a_G^{(+)}(\mathbf{q}; t). \quad (16.142)$$

It is obvious that this choice does satisfy the constraint in (16.137) because $a_G^{(+)}(\mathbf{q}; t)$ fulfils the quantum mechanical wave equation in (16.126). The transformation given by the $f^{(+)}(\mathbf{q}; t)$ in (16.142), therefore, is a gauge transformation *within* the Lorenz gauge. By inserting (16.142) into (16.140) it appears that

$$a_G^{(+)\text{NEW}}(\mathbf{q}; t) = (2c_0 q)^{-1} (c_0 q - i \frac{\partial}{\partial t}) a_G^{(+)}(\mathbf{q}; t). \quad (16.143)$$

The dynamical equation for the gauge photon wave function in (16.126) in turn gives

$$a_G^{(+)\text{NEW}}(\mathbf{q}; t) = 0. \quad (16.144)$$

In free space, the gauge photon hence can be eliminated by a suitable gauge transformation within the Lorenz gauge.

Starting with the introduction of longitudinal and scalar photons we have realized that the net physical effect of these photons vanishes in free space, because the two photon types have identical quantum mechanical wave functions. For near-field electrodynamics the longitudinal part of the electric field plays a particular role, and this makes it suitable to introduce two new photon types, the gauge and near-field photon. In free space, the near-field photon wave function is identically zero, and the gauge photon wave function can be eliminated by a suitable gauge transformation within the Lorenz gauge.

Chapter 17

Photon Angular Momentum

In several paragraphs that precede this chapter, we have studied aspects related to the angular momentum of the electromagnetic field. Thus, in the framework of the microscopic theory of classical electrodynamics the global (Sect. 2.6.3) and local (Sect. 2.7.4) angular momenta of the field were discussed, and the angular momentum flow associated with particle interactions analyzed. In our treatment of transverse electromagnetic multipole waves (Sect. 5.4), further insight was obtained from a study of the differential equation which spherical harmonics satisfy. In an Interlude (Sect. 5.4.2), the classical angular field momentum operator was introduced, and related to the angular momentum operator appearing in the quantum theory of massive particles. An important step forward in our understanding of the structure of the field angular momentum was taken in Sect. 9.3.4. There it was shown that the part of the classical field momentum which contains the longitudinal electric field can be considered as a contribution to the particle orbital angular momentum. The remaining part, associated to the transverse electric field, viz.,

$$\mathbf{J} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{r} \times (\mathbf{E}_T(\mathbf{r}, t) \times \mathbf{B}(\mathbf{r}, t)) d^3r \quad (17.1)$$

is the one which relates to the dynamical variables of the electromagnetic field. In free space, where $\mathbf{E}_L(\mathbf{r}, t) = \mathbf{0}$, $\mathbf{J}$ is a conserved quantity. The expression in (17.1) is closely connected to the angular momentum of the photon in wave mechanics, and we have therefore used the symbol $\mathbf{J}$ instead of $\mathbf{I}_{\text{trans}}$ (9.95) to denote the angular momentum of the transverse electromagnetic field. In our discussion of the complex field theory in the space–time domain a Cartesian photon spin operator was introduced (Sect. 15.5.1). The same operator also appeared in the photon energy wave function formalism (compare (15.111) and (16.25)). In this chapter, a more detailed analysis of the photon angular momentum is presented.

17.1 Bodily Rotation of Scalar and Vector Fields

We begin with some considerations which at first sight may appear quite remote from the main theme, viz., the classification of general scalar and vector fields according to their behavior in spatial rotations about some fixed axis.

Suppose that a given *scalar* field $A(\mathbf{r})$ is described relative to a Cartesian frame centered on the axis of rotation. A bodily rotation replaces the field $A(\mathbf{r})$ in the space point $\mathbf{r}$ by $A'(\mathbf{r}) = A(\mathbf{r} - \delta\mathbf{r})$, where

$$\delta\mathbf{r} = \delta\boldsymbol{\alpha} \times \mathbf{r}. \quad (17.2)$$

The vector $\delta\boldsymbol{\alpha}$ characterizes the bodily rotation in the usual manner: $|\delta\boldsymbol{\alpha}|$ is the magnitude of the rotation angle, and $\delta\boldsymbol{\alpha}/|\delta\boldsymbol{\alpha}|$ is a unit vector along the axis of rotation. The rotation angle is counted positive if the rotation is counterclockwise as seen against the direction of $\delta\boldsymbol{\alpha}/|\delta\boldsymbol{\alpha}|$. The change in the scalar field at $\mathbf{r}$, hence is given by

$$\delta A(\mathbf{r}) \equiv A(\mathbf{r} - \delta\boldsymbol{\alpha} \times \mathbf{r}) - A(\mathbf{r}). \quad (17.3)$$

In the limit of an infinitesimal rotation ($|\delta\boldsymbol{\alpha}| \rightarrow 0$), one has to first order

$$\delta A(\mathbf{r}) = -(\delta\boldsymbol{\alpha} \times \mathbf{r}) \cdot \nabla A(\mathbf{r}) = -i\delta\boldsymbol{\alpha} \cdot \hat{\mathbf{L}} A(\mathbf{r}), \quad (17.4)$$

where

$$\hat{\mathbf{L}} = -i\mathbf{r} \times \nabla \quad (17.5)$$

is the (dimensionless) orbital angular momentum operator. The quantity $\hbar\hat{\mathbf{L}}$ may be recognized by the reader as the particle orbital angular momentum in quantum mechanics. In the language of group theory, one says that $\hat{\mathbf{L}}$ is the generator of infinitesimal spatial rotations.

Before proceeding the analysis of body rotations it is useful briefly to consider the bodily *translation* of the field $A(\mathbf{r})$. For a translation $\delta\mathbf{r}$, one obtains in the limit $|\delta\mathbf{r}| \rightarrow 0$ a change in the field description at $\mathbf{r}$

$$\delta A(\mathbf{r}) = -\delta\mathbf{r} \cdot \nabla A(\mathbf{r}) = -i\delta\mathbf{r} \cdot \hat{\mathbf{P}} A(\mathbf{r}), \quad (17.6)$$

where the momentum operator

$$\hat{\mathbf{P}} = -i\nabla \quad (17.7)$$

appears as the generator of infinitesimal spatial translations. The quantity $\hbar\hat{\mathbf{P}}$ is the well known momentum operator in quantum mechanics.

Let us now consider the bodily rotation of a *vector* field $\mathbf{A}(\mathbf{r})$, and let the operation be characterized by a rotation matrix $\mathbf{R}$. The field vector which *after* the rotation ends up at the space point $\mathbf{r}$, *before* the rotation was located at the point $\mathbf{R}^{-1} \cdot \mathbf{r}$ ($\mathbf{R}^{-1}$ being the inverse rotation matrix to $\mathbf{R}$). Upon rotation the vector field $\mathbf{A}(\mathbf{R}^{-1} \cdot \mathbf{r})$ originally located at $\mathbf{R}^{-1} \cdot \mathbf{r}$ is changed (rotated) into $\mathbf{R} \cdot \mathbf{A}(\mathbf{R}^{-1} \cdot \mathbf{r})$. The change in the vector field at $\mathbf{r}$, thus is given by

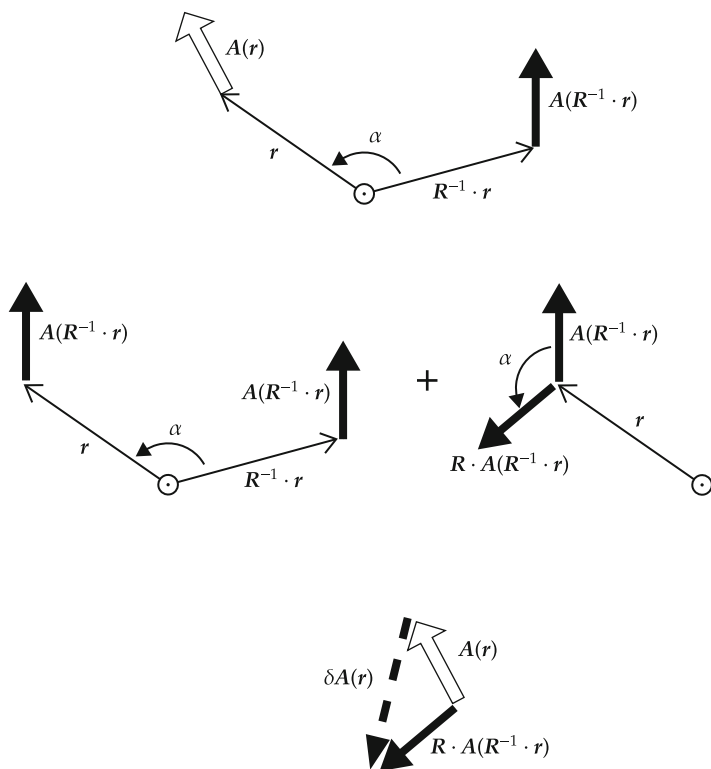


Fig. 17.1 Bodily rotation of a vector field $A(\mathbf{r})$, through an angle α , around an axis perpendicular to the plane of the paper. *Top figure*: By means of the rotation matrix $\mathbf{R}$ a vector $A(\mathbf{R}^{-1} \cdot \mathbf{r})$ (black arrow) located at $\mathbf{R}^{-1} \cdot \mathbf{r}$ is rotated to the position $\mathbf{r}$. Before the rotation the vector at $\mathbf{r}$ was $A(\mathbf{r})$ (white arrow). *Middle figures*: The bodily rotation is done in two steps. (1) The field point $\mathbf{R}^{-1} \cdot \mathbf{r}$ is rotated into $\mathbf{r}$ without changing the vector $A(\mathbf{R}^{-1} \cdot \mathbf{r})$. (2) To preserve the angle between the position and field vectors, one must (at $\mathbf{r}$) rotate the vector $A(\mathbf{R}^{-1} \cdot \mathbf{r})$ an angle α . *Bottom figure*: The bodily rotation results in a change $\delta A(\mathbf{r}) = \mathbf{R} \cdot A(\mathbf{R}^{-1} \cdot \mathbf{r}) - A(\mathbf{r})$ in the vector field at $\mathbf{r}$

$$\delta A(\mathbf{r}) = \mathbf{R} \cdot A(\mathbf{R}^{-1} \cdot \mathbf{r}) - A(\mathbf{r}). \quad (17.8)$$

Upon a comparison of (17.3) and (17.8) it appears that the bodily rotation of a vector field $[A(\mathbf{r})]$ is somewhat more complicated to characterize than that of a scalar field $[A(\mathbf{r})]$ due to the fact that not only is its dependence on the field point changed, as for a scalar field, but also the direction of the field vector is changed in the various space points; cf. Fig. 17.1.

To determine the generator of the infinitesimal vector field rotations we first consider a rotation about the z -axis of our Cartesian coordinate system. A counterclockwise rotation by an angle α is characterized by a rotation matrix

$$\mathbf{R}(\alpha) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (17.9)$$

and if the rotation is infinitesimal ($\alpha \rightarrow \delta\alpha \rightarrow 0$) one has in first order

$$\mathbf{R}(\delta\alpha) = \begin{pmatrix} 1 & -\delta\alpha & 0 \\ \delta\alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (17.10)$$

and thus (with $\delta\alpha$ replaced by $-\delta\alpha$)

$$\mathbf{R}^{-1} \cdot \mathbf{r} = \begin{pmatrix} 1 & \delta\alpha & 0 \\ -\delta\alpha & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x + y\delta\alpha \\ y - x\delta\alpha \\ z \end{pmatrix}. \quad (17.11)$$

A Taylor series expansion of the vector field $\mathbf{A}(\mathbf{R}^{-1} \cdot \mathbf{r})$ to first order around $\mathbf{r} = (x, y, z)$ therefore gives

$$\begin{aligned} \mathbf{A}(\mathbf{R}^{-1} \cdot \mathbf{r}) &\cong \mathbf{A}(x + y\delta\alpha, y - x\delta\alpha, z) \\ &\cong \mathbf{A}(\mathbf{r}) - \delta\alpha \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \mathbf{A}(\mathbf{r}) \\ &= \mathbf{A}(\mathbf{r}) - \delta\alpha (\mathbf{r} \times \nabla)_z \mathbf{A}(\mathbf{r}), \end{aligned} \quad (17.12)$$

and hereafter

$$\mathbf{R} \cdot \mathbf{A}(\mathbf{R}^{-1} \cdot \mathbf{r}) \cong \mathbf{R} \cdot \mathbf{A}(\mathbf{r}) - \delta\alpha (\mathbf{r} \times \nabla)_z \mathbf{R} \cdot \mathbf{A}(\mathbf{r}). \quad (17.13)$$

By now, we just need to determine the action of the infinitesimal rotation matrix in (17.10) on $\mathbf{A}(\mathbf{r})$. Matrix multiplication immediately leads to

$$\mathbf{R}(\delta\alpha) \cdot \mathbf{A}(\mathbf{r}) = \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} + \delta\alpha \begin{pmatrix} -A_y \\ A_x \\ 0 \end{pmatrix}, \quad (17.14)$$

or equivalently

$$\mathbf{R}(\delta\alpha) \cdot \mathbf{A}(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \delta\alpha \hat{\mathbf{z}} \times \mathbf{A}(\mathbf{r}). \quad (17.15)$$

By combining (17.13) and (17.15), and keeping (consistently) only terms to first-order in $\delta\alpha$, one obtains the following expression for the change (17.8) in the vector field:

$$\delta \mathbf{A}(\mathbf{r}) = -i\delta\alpha [-i(\mathbf{r} \times \nabla)_z \mathbf{A}(\mathbf{r}) + i\hat{\mathbf{z}} \times \mathbf{A}(\mathbf{r})]. \quad (17.16)$$

In Sect. 15.5.1, we introduced the Cartesian photon spin operator, $\hat{s}$. The related dimensionless spin operator

$$\hat{S} \equiv \hbar^{-1} \hat{s} \quad (17.17)$$

enters the description of the bodily rotation of a vector field. Thus, by means of the matrix representation of the z -component of $\hat{S}$, one may write

$$i\hat{z} \times \mathbf{A}(\mathbf{r}) = \hat{S}_z \cdot \mathbf{A}(\mathbf{r}), \quad (17.18)$$

and in a slightly compressed notation we finally get by use of (17.5) and (17.18)

$$\delta \mathbf{A}(\mathbf{r}) = -i\delta\alpha(\hat{L}_z + \hat{S}_z)\mathbf{A}(\mathbf{r}). \quad (17.19)$$

This result shows that the generator of infinitesimal rotation of a vector field around the z -axis is the sum of the z -components of the (dimensionless) orbital and spin angular momentum operators. In going from rotations of scalar (17.4) to vector (17.19) fields a spin term emerges. The finding in (17.19) is generalizable to infinitesimal rotations ($\delta\alpha$) about an arbitrary axis:

$$\delta \mathbf{A}(\mathbf{r}) = -i(\delta\alpha \cdot \hat{\mathbf{J}})\mathbf{A}(\mathbf{r}), \quad (17.20)$$

where

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}} \quad (17.21)$$

is the sum of the (dimensionless) orbital and spin angular momentum operators.

17.2 Orbital and Spin Parts of the Photon Angular Momentum

17.2.1 Division of the Angular Momentum of the Transverse Electromagnetic Field

In Sect. 9.3.4, we examined the part of the field angular momentum which contains the longitudinal electric field. Starting from (9.83) we proceeded to the expression given in (9.87) for $\mathbf{I}_{\text{long}}$. By a comparison of (9.83) [$\mathbf{I}_{\text{long}}$] and (17.1) [$\hat{\mathbf{J}}$], it appears that we can obtain an expression for $\hat{\mathbf{J}}$ similarly to the one the right side of (9.87) just by replacing $\mathbf{E}_L$ by $\mathbf{E}_T$. If one then takes into account the fact that $\nabla \cdot \mathbf{E}_T = 0$ the last of the three terms in the integrand vanishes. In a classical perspective, the angular momentum of the transverse electromagnetic field thus is the sum of the two parts, viz.,

$$\mathbf{J} = \mathbf{L} + \mathbf{S}, \quad (17.22)$$

where

$$\mathbf{L} = \epsilon_0 \sum_i \int_{-\infty}^{\infty} \mathbf{E}_{T,i}(\mathbf{r}, t)(\mathbf{r} \times \nabla) A_{T,i}(\mathbf{r}, t) d^3 r, \quad (17.23)$$

and

$$\mathbf{S} = \epsilon_0 \int_{-\infty}^{\infty} \mathbf{E}_T(\mathbf{r}, t) \times \mathbf{A}_T(\mathbf{r}, t) d^3 r. \quad (17.24)$$

The $\mathbf{L}$ -term is called the orbital angular momentum of the transverse field. This part depends on the reference point chosen, here the origo $\mathbf{r} = \mathbf{0}$, and is denoted by $\mathbf{L}(\mathbf{0})$. If the reference point is $\mathbf{r} = \mathbf{r}_0$, the corresponding orbital angular momentum is denoted by $\mathbf{L}(\mathbf{r}_0)$. Since the $\mathbf{S}$ -term is independent of the choice of reference point, as one can readily see from (17.24), the reader may easily convince himself beginning with (17.1) and using (9.81) that

$$\mathbf{L}(\mathbf{r}_0) = \mathbf{L}(\mathbf{0}) - \mathbf{r}_0 \times \mathbf{P}_{\text{trans}}. \quad (17.25)$$

Although we have not referred to single-photon fields above, the designations $\mathbf{L}$ and $\mathbf{S}$ have been used for the two parts of the transverse electromagnetic field. In free space the total angular field momentum is conserved, i.e.,

$$\frac{d\mathbf{J}}{dt} = \mathbf{0}, \quad (17.26)$$

cf. the analysis in Sect. 2.6.3. In the context of the discussion of the bodily vector field rotation given in Sect. 17.1, (17.26) also follows from the invariance of the Maxwell equations under spatial rotations.

The $\mathbf{S}$ -term, given in (17.24), is manifestly independent of the choice of reference point, as already stated, and it is called the spin contribution to the angular momentum of the transverse electromagnetic field. Since only the transverse part of the vector potential enters the expressions for $\mathbf{L}$ and $\mathbf{S}$, the two contributions are both gauge independent. That the total angular momentum $\mathbf{J}$ is gauge independent is obvious from (17.1). Let us now prove that $\mathbf{S}$ is a time-conserved quantity for a free field. By differentiation of (17.24) with respect to time one obtains

$$\frac{d\mathbf{S}}{dt} = \epsilon_0 \int_{-\infty}^{\infty} \frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{r}, t) \times \mathbf{A}_T(\mathbf{r}, t) d^3 r, \quad (17.27)$$

since $\mathbf{E}_T \times \partial \mathbf{A} / \partial t = -\mathbf{E}_T \times \mathbf{E}_T = \mathbf{0}$. Next, the transverse electric field is eliminated from (17.27) utilizing the relation

$$\frac{\partial}{\partial t} \mathbf{E}_T(\mathbf{r}, t) = -\frac{\partial^2}{\partial t^2} \mathbf{A}_T(\mathbf{r}, t) = -c_0 \nabla^2 \mathbf{A}_T(\mathbf{r}, t). \quad (17.28)$$

The last step in (17.28) follows from the wave equation for the transverse vector potential in the free space. Hence, we find

$$\frac{d\mathbf{S}}{dt} = \frac{1}{\mu_0} \int_{-\infty}^{\infty} \mathbf{A}_T(\mathbf{r}, t) \times \nabla^2 \mathbf{A}_T(\mathbf{r}, t) d^3 r. \quad (17.29)$$

Partial integrations, and use of the fact that the field is only nonvanishing in a finite region of space (disregard of surface terms at infinity), next gives [$i = (x, y, z)$]

$$\frac{dS}{dt} = - \sum_i \int_{-\infty}^{\infty} \frac{\partial}{\partial i} A_T(\mathbf{r}, t) \times \frac{\partial}{\partial i} A_T(\mathbf{r}, t) d^3r = \mathbf{0}, \quad (17.30)$$

the result we promised to prove. Since the total angular momentum and its spin part both are conserved ((17.26) and (17.30)), also the orbital angular momentum of the electromagnetic field in free space must be conserved in time, i.e.,

$$\frac{dL}{dt} = \mathbf{0} \quad (17.31)$$

In preparation of the analysis of the photon angular momentum in wave mechanics it is useful to express the two contributions to the angular momentum of the free electromagnetic field in the form of integrals over reciprocal space. For the spin part (17.24) the Parseval–Plancherel identity immediately gives

$$S = \epsilon_0 \int_{-\infty}^{\infty} E_T^*(\mathbf{q}; t) \times A_T(\mathbf{q}; t) \frac{d^3q}{(2\pi)^3}. \quad (17.32)$$

In order to use this identity in the expression for the orbital angular momentum (17.23) one needs the Fourier integral transform of the quantity $(\mathbf{r} \times \nabla) A_{T,i}(\mathbf{r}, t)$. With the operator transformations $\nabla \Rightarrow i\mathbf{q}$, and $\mathbf{r} \Rightarrow i\nabla_{\mathbf{q}}$, one finds the connection

$$\mathbf{r} \times \nabla(\dots) \Rightarrow -\nabla_{\mathbf{q}} \times [\mathbf{q}(\dots)] = \mathbf{q} \times \nabla_{\mathbf{q}}(\dots), \quad (17.33)$$

where the last expression follows from the fact that $\nabla_{\mathbf{q}} \times \mathbf{q} = \mathbf{0}$. The Parseval–Plancherel identity applied to (17.23) therefore gives

$$L = \epsilon_0 \sum_i \int_{-\infty}^{\infty} E_{T,i}^*(\mathbf{q}; t) (\mathbf{q} \times \nabla_{\mathbf{q}}) A_{T,i}(\mathbf{q}; t) \frac{d^3q}{(2\pi)^3}. \quad (17.34)$$

17.2.2 *Quantum Mechanical Mean Values of the Orbital and Spin Angular Momenta in the Complex Field Theory*

The classical theory of the angular momentum of the field is translated to photon wave mechanics by making the usual replacements $E_T(\mathbf{q}; t) \Rightarrow e_T^{(+)}(\mathbf{q}; t)$ and $A_T(\mathbf{q}; t) \Rightarrow a_T^{(+)}(\mathbf{q}; t)$ in (17.32) and (17.34). By denoting also the single-photon orbital and spin angular momenta by L and S , respectively, we have

$$\mathbf{L} = \epsilon_0 \sum_i \int_{-\infty}^{\infty} [e_{T,i}^{(+)}(\mathbf{q}; t)]^* (\mathbf{q} \times \nabla_{\mathbf{q}}) a_{T,i}^{(+)}(\mathbf{q}; t) \frac{d^3 q}{(2\pi)^3}, \quad (17.35)$$

and

$$\mathbf{S} = \epsilon_0 \sum_i \int_{-\infty}^{\infty} [e_T^{(+)}(\mathbf{q}; t)]^* \times a_T^{(+)}(\mathbf{q}; t) \frac{d^3 q}{(2\pi)^3}. \quad (17.36)$$

It is possible to show that the angular momenta $\mathbf{L}$ and $\mathbf{S}$ can be expressed as quantum mechanical mean values of certain characteristic operators. Below we shall briefly discuss these mean value forms in the complex field theory as well as in the energy wave function formalism. For brevity, certain steps are omitted in our proceedings from (17.35) and (17.36) to the final formulas.

In the complex field theory the analytical electric field $e_T^{(+)}(\mathbf{q}; t)$ is related to the vectorial photon wave functions $\beta_{\pm}^{(+)}(\mathbf{q}; t)$ via (15.83). To obtain the relation between the analytical vector potential $a_T^{(+)}(\mathbf{q}; t)$ and the $\beta_{\pm}^{(+)}(\mathbf{q}; t)$'s we multiply the two sides of (16.82) vectorially from the left with $\hat{\mathbf{q}}$. This gives the following expression for $a_T^{(+)}(\mathbf{q}; t)$:

$$a_T^{(+)}(\mathbf{q}; t) = \frac{i}{q} \hat{\mathbf{q}} \times \mathbf{b}^{(+)}(\mathbf{q}; t). \quad (17.37)$$

If one in this equation inserts the expression for $\mathbf{b}^{(+)}(\mathbf{q}; t)$ given in (15.84) one gets

$$a_T^{(+)}(\mathbf{q}; t) = (2\pi)^{3/2} \frac{N\beta(q)}{2c_0 q} \hat{\mathbf{q}} \times (\beta_+^{(+)}(\mathbf{q}; t) - \beta_-^{(+)}(\mathbf{q}; t)). \quad (17.38)$$

By means of (15.71) and (15.72) it is easy to show that

$$e_T^{(+)}(\mathbf{q}; t) = i c_0 q a_T^{(+)}(\mathbf{q}; t). \quad (17.39)$$

When the expressions for $e_T^{(+)}(\mathbf{q}; t)$ (15.83) and for $a_T^{(+)}(\mathbf{q}; t)$, taken from (17.39), are inserted in (17.35) and (17.36) the orbital and spin angular momenta of the photon are given in terms of certain integrals involving only bilinear combinations of the photon wave functions $\beta_{\pm}^{(+)}(\mathbf{q}; t)$. It is possible to prove [180] that cross terms involving opposite helicity states do not contribute to the orbital angular momentum that is

$$\int_{-\infty}^{\infty} [\beta_{\pm,i}^{(+)}(\mathbf{q}; t)]^* (\mathbf{q} \times \nabla_{\mathbf{q}}) \beta_{\mp,i}^{(+)}(\mathbf{q}; t) d^3 q = 0 \quad (17.40)$$

for all i . With the result in (17.40) established, elementary calculations lead to the expression

$$\mathbf{L} = \sum_i \int_{-\infty}^{\infty} \sum_{s=+,-} [\beta_{s,i}^{(+)}(\mathbf{q}; t)]^* \hat{\ell}(\mathbf{q}) \beta_{s,i}^{(+)}(\mathbf{q}; t) d^3 q, \quad (17.41)$$

where

$$\hat{\ell}(\mathbf{q}) = i \nabla_{\mathbf{q}} \times (\hbar \mathbf{q}) = -i \hbar \mathbf{q} \times \nabla_{\mathbf{q}}. \quad (17.42)$$

Since $\hat{\ell}(\mathbf{q})$ is just the particle angular momentum operator in the reciprocal-space representation, the orbital angular momentum of the photon field in (17.41) appears in the standard quantum mechanical mean value form. With the translations $\mathbf{r} \Rightarrow i \nabla_{\mathbf{q}}$ and $\nabla \Rightarrow i \mathbf{q}$ in (17.5) one obtains the expected result

$$\hat{\ell}(\mathbf{q}) = \hbar \hat{L}(\mathbf{q}). \quad (17.43)$$

Let us turn our attention towards the spin contribution to the photon angular momentum. Also in the spin case it is possible to show [180] that cross terms related to opposite helicity states do not contribute to $\mathbf{S}$. Once this has been realized it is easy to demonstrate that the spin of the photon field is given by the integral expression

$$\mathbf{S} = \int_{-\infty}^{\infty} \frac{\hbar}{i} \sum_{s=+,-} \left[\beta_s^{(+)}(\mathbf{q}; t) \right]^* \times \beta_s^{(+)}(\mathbf{q}; t) d^3 q. \quad (17.44)$$

A further simplification is obtained by utilizing (15.71) and (15.91). Thus,

$$\mathbf{S} = \int_{-\infty}^{\infty} \hbar \hat{\mathbf{q}} \left(|\beta_+^{(+)}(\mathbf{q}; t)|^2 - |\beta_-^{(+)}(\mathbf{q}; t)|^2 \right) d^3 q. \quad (17.45)$$

It appears from (17.45) that a photon which is in an eigenstate for the momentum (with wave vector $\mathbf{q}_0$, say) has a spin $\hbar \hat{\mathbf{q}}_0$ if it has positive helicity, and a spin $-\hbar \hat{\mathbf{q}}_0$ if its helicity is negative. In the spinorial representation the spin of the photon field is given by the compact formula

$$\mathbf{S} = \int_{-\infty}^{\infty} \hbar \hat{\mathbf{p}} (\Phi^{\text{CF}}(\mathbf{p}; t))^{\dagger} \cdot \begin{pmatrix} U & \mathbf{0} \\ \mathbf{0} & U \end{pmatrix} \cdot \Phi^{\text{CF}}(\mathbf{p}; t) d^3 p. \quad (17.46)$$

in the framework of the complex field theory.

17.2.3 *Quantum Mechanical Mean Values of the Orbital and Spin Angular Momenta in the Energy Wave Function Formalism*

In the Riemann–Silberstein approach to classical electromagnetics in free space, the angular momentum of the transverse field was given by (16.18), possibly with $\mathbf{F}_-(\mathbf{r}, t)$ replaced by $\mathbf{F}_+^*(\mathbf{r}, t)$, cf. (16.5). By means of the formula $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$ it is not difficult to show that the total angular momentum of the single-photon field may be written as follows:

$$\mathbf{J} = \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{f}_+^*(\mathbf{r}, t) (\mathbf{r} \cdot \mathbf{f}_+(\mathbf{r}, t)) d^3r + c.c., \quad (17.47)$$

where $\mathbf{f}_+ = \mathbf{f}_+^{(+)} + \mathbf{f}_-^{(+)}$ is the sum of the photon energy wave functions for the two helicity species. A tedious calculation [180] learns us that the orbital angular momentum of the photon can be expressed in the quantum mechanical mean value form

$$\mathbf{L} = \frac{1}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \left[f_s^{(+)}(\mathbf{q}, c_0 q) \right]^* [-i\hbar \mathbf{q} \times \mathbf{D}_{q,s}] f_s^{(+)}(\mathbf{q}, c_0 q) \frac{d^3q}{(2\pi)^3 q}, \quad (17.48)$$

where, with $\eta_+ = 1$ and $\eta_- = -1$,

$$\mathbf{D}_{q,s} = \nabla_q + i\eta_s \boldsymbol{\alpha}(\hat{\mathbf{q}}) \quad (17.49)$$

is the so-called natural covariant derivative on the light cone [213]. The vector $\boldsymbol{\alpha}(\hat{\mathbf{q}})$ is conveniently given in terms of a set of two real unit polarization vectors, cf. (15.49)–(15.51):

$$\boldsymbol{\alpha}(\hat{\mathbf{q}}) = \hat{\boldsymbol{\epsilon}}_1^R(\hat{\mathbf{q}}) \cdot \nabla_q \hat{\boldsymbol{\epsilon}}_2^R(\hat{\mathbf{q}}) - \hat{\boldsymbol{\epsilon}}_2^R(\hat{\mathbf{q}}) \cdot \nabla_q \hat{\boldsymbol{\epsilon}}_1^R(\hat{\mathbf{q}}). \quad (17.50)$$

In (17.48), the crossproduct $\mathbf{q} \times \boldsymbol{\alpha}(\hat{\mathbf{q}})$ appears, and when evaluating this product it is understood that one *first* forms the vectorial products $\mathbf{q} \times \hat{\boldsymbol{\epsilon}}_1^R$ and $\mathbf{q} \times \hat{\boldsymbol{\epsilon}}_2^R$, and *then* makes the scalar products with ∇_q . In terms of helicity unit vectors one has

$$\mathbf{q} \times \boldsymbol{\alpha}(\hat{\mathbf{q}}) = (\hat{\mathbf{e}}_+ \cdot \nabla_q) \hat{\mathbf{e}}_+^* + (\hat{\mathbf{e}}_+^* \cdot \nabla_q) \hat{\mathbf{e}}_+. \quad (17.51)$$

The reader may show that $\boldsymbol{\alpha}(\hat{\mathbf{q}})$ depends on the *chosen* set of real unit polarization vectors, and thus on the *overall* phase convention for the helicity unit vectors. The spin part of the angular photon momentum has the integral representation

$$\mathbf{S} = \frac{1}{\hbar c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \left[f_s^{(+)}(\mathbf{q}, c_0 q) \right]^* [\eta_s \hbar \hat{\mathbf{q}}] f_s^{(+)}(\mathbf{q}, c_0 q) \frac{d^3q}{(2\pi)^3 q} \quad (17.52)$$

in the energy wave function theory.

17.3 More on the Photon Spin and Helicity

17.3.1 Are $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$ Separate Observables for a Photon?

In Sect. 17.1, we analyzed the bodily rotation of a vector field in direct space. An analogous analysis can of course be carried out for vector fields defined in reciprocal

space. The change in the vector field $\mathbf{A}(\mathbf{q})$ thus is given by

$$\delta \mathbf{A}(\mathbf{q}) = \mathbf{R}_q \cdot \mathbf{A} \left(\mathbf{R}_q^{-1} \cdot \mathbf{q} \right) - \mathbf{A}(\mathbf{q}), \quad (17.53)$$

where $\mathbf{R}_q$ is the relevant rotation matrix in $\mathbf{q}$ -space. In the photon case, $\mathbf{A}(\mathbf{q})$ must be a transverse vector, i.e., the condition $\mathbf{q} \cdot \mathbf{A}(\mathbf{q}) = 0$ always has to be satisfied. The orbital angular momentum operator in $\mathbf{q}$ -space, namely

$$\hat{\mathbf{L}}(\mathbf{q}) = -i \mathbf{q} \times \nabla_q, \quad (17.54)$$

is associated with a rotation of the field point $\mathbf{q}$ for each vector $\mathbf{A}(\mathbf{q})$. In such a rotation, where the direction of the vector field $\mathbf{A}$ is unchanged, the orthogonality between the vectors $\mathbf{q}$ and $\mathbf{A}(\mathbf{q})$ is *not* conserved. In the language of quantum mechanics, an infinitesimal rotation defined by the orbital angular momentum generator in (17.54) thus brings the photon wave function outside the subspace of transverse vector fields. The spin operator $\mathbf{S}$ gives rise to a rotation of the vector field $\mathbf{A}(\mathbf{q})$, but the field point $\mathbf{q}$ is unchanged. An infinitesimal rotation defined by the spin angular momentum operator therefore also causes a break down of the transversality condition. Only rotations defined by the generator $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ preserve angles, and allows the photon wave function to stay in the subspace of transverse vector fields.

In the context of relativity, the spin of a particle represents its total angular momentum observed in a frame where it is instantaneously at rest. For a photon, which necessarily propagates with the vacuum speed of light, such a frame does not exist.

17.3.2 Quantum Mechanical Mean Value of the Cartesian Photon Spin Operator

In Sect. 17.2.2, the complex field theory allowed us to express the spin of the photon field in the form of a characteristic integral over reciprocal space (17.45). In Sect. 17.2.3, we gave within the framework of the energy wave function formalism another $\mathbf{q}$ -space integral for the spin of the photon (17.52). At first sight the expressions in (17.45) and (17.52) seem to have slightly different structural forms, but if one introduces the scaled scalar wave functions

$$g_{\pm}(\mathbf{q}; t) = (2\pi)^{-3/2} (c_0 \hbar q)^{-1/2} f_{\pm}^{(+)}(\mathbf{q}; t) \quad (17.55)$$

in (17.52) one obtains

$$\mathbf{S} = \int_{-\infty}^{\infty} \hbar \hat{\mathbf{q}} \left(|g_+(\mathbf{q}; t)|^2 - |g_-(\mathbf{q}; t)|^2 \right) d^3 q. \quad (17.56)$$

The structural forms of the $\mathbf{q}$ -space integrals for the spin of the photon field now appear identical in the two formulations of photon wave mechanics. The reader may recall that the scaled wave functions in (17.55) already have been used in Sect. 16.1.3 in relation to the discussion of the quantum mechanical mean value of the energy–momentum operator; see in particular (16.44), (16.45), and (16.59).

In Sect. 15.5.1, the Cartesian photon spin operator $\hat{\mathbf{s}} = (\hat{s}_x, \hat{s}_y, \hat{s}_z)$ was introduced. We shall now show that the spin of the photon field (in both theories) is equal to the quantum mechanical mean value of this spin-one particle operator. In order to make the bridge from (17.56) (or (17.45)) to an expression containing the particle spin operator in (15.99) one utilizes the following central equation:

$$\hat{\mathbf{e}}_{\pm}^{\dagger}(\hat{\mathbf{q}}) \cdot \mathbf{s}_i \cdot \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) = -i\hbar (\hat{\mathbf{e}}_{\pm}^*(\hat{\mathbf{q}}) \times \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}))_i. \quad (17.57)$$

Before proceeding let us clarify the notation used in this equation. On the left side appears a matrix product: The matrix representative of the i th component ($i = x, y, z$) of the spin operator thus is multiplied from the right by the column vector $\hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}})$ and from the left with this vectors complex conjugate row vector $\hat{\mathbf{e}}_{\pm}^{\dagger}$. On the right side of (17.57) we have the i th component of the vectorial product of $\hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}})$ and its complex conjugate. The Cartesian representatives of the $\mathbf{s}_i$'s are given in (15.100)–(15.102), and with $\mathbf{e}_{\pm} = (e_{\pm,x}, e_{\pm,y}, e_{\pm,z})$ straightforward calculations prove the assertion in (17.57). By means of (15.91) we next realize that

$$\hat{\mathbf{e}}_{\pm}^{\dagger}(\hat{\mathbf{q}}) \cdot \mathbf{s}_i \cdot \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) = \pm\hbar(\hat{\mathbf{q}})_i, \quad (17.58)$$

where $(\hat{\mathbf{q}})_i$ is the i th component of the unit vector $\hat{\mathbf{q}}$. Let us now utilize (17.58) in a rewriting of (17.56). Multiplication of (17.58) by $|g_{\pm}|^2 = g_{\pm}^* g_{\pm}$ gives

$$g_{\pm}^*(\mathbf{q}; t) \hat{\mathbf{e}}_{\pm}^{\dagger}(\hat{\mathbf{q}}) \cdot \mathbf{s}_i \cdot \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) g_{\pm}(\mathbf{q}; t) = \pm\hbar(\hat{\mathbf{q}})_i |g_{\pm}(\mathbf{q}; t)|^2, \quad (17.59)$$

and with the notation

$$\mathbf{g}_{\pm}(\mathbf{q}; t) = g_{\pm}(\mathbf{q}; t) \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) = (2\pi)^{-3/2} (c_0 \hbar q)^{-1/2} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) \quad (17.60)$$

it is obvious that the i th component of the spin of the photon field can be written in the form

$$S_i = \sum_{s=+,-} \int_{-\infty}^{\infty} \mathbf{g}_s^{\dagger}(\mathbf{q}; t) \cdot \mathbf{s}_i \cdot \mathbf{g}_s(\mathbf{q}; t) d^3 q. \quad (17.61)$$

With the compact notation

$$(\mathbf{g}_s^{\dagger} \hat{\mathbf{s}} \mathbf{g}_s)_i \equiv \mathbf{g}_s^{\dagger} \cdot \mathbf{s}_i \cdot \mathbf{g}_s, \quad (17.62)$$

the spin of the photon field ($\mathbf{S}$) finally appears as the quantum mechanical mean value of the Cartesian spin-one operator, $\hat{\mathbf{s}}$, i.e.,

$$\mathbf{S} = \sum_{s=+,-} \int_{-\infty}^{\infty} \mathbf{g}_s^\dagger(\mathbf{q}; t) \hat{\mathbf{s}} \mathbf{g}_s(\mathbf{q}; t) d^3q. \quad (17.63)$$

The result in (17.63) refers to the energy wave function formalism. The corresponding result in the complex field theory follows upon the substitution $\mathbf{g}_s(\mathbf{q}; t) \Rightarrow \boldsymbol{\beta}_s^{(+)}(\mathbf{q}; t)$.

17.3.3 Projected Photon Spin Operator

The photon spin operator $\hat{\mathbf{s}}$ in a sense is a genuine angular momentum operator because it satisfies the vectorial commutator relation $\hat{\mathbf{s}} \times \hat{\mathbf{s}} = i\hbar \hat{\mathbf{s}}$. In fact, it is the form of this relation which defines $\hat{\mathbf{s}}$ as an angular momentum operator in quantum mechanics. Putting aside for a moment the reality that no observations can separate the orbital and spin angular momenta of the photon from each other, the three Cartesian components of the spin are not as such simultaneously observable because the related operators do not commute. As we shall realize below, it is however possible to replace the spin operator in (17.63) by another operator which quantum mechanical mean value also equals the spin ($\mathbf{S}$) of the photon field. The new operator, called the projected spin operator and denoted by $\hat{\mathbf{s}}^{\text{proj}}$, has commuting components. Since $\hat{\mathbf{s}}^{\text{proj}}$ thus does not satisfy the vectorial commutator relation which defines an orbital angular momentum operator in quantum mechanics, its three Cartesian components are simultaneously measurable (forgetting again the fundamental impossibility of distinguishing uniquely $\mathbf{L}$ and $\mathbf{S}$ for the photon field).

The transverse nature of the photon wave functions $\mathbf{g}_s(\mathbf{q}; t)$ [$s = +, -$] implies that

$$\mathbf{g}_s(\mathbf{q}; t) = (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{g}_s(\mathbf{q}; t). \quad (17.64)$$

By inserting this identity into (17.63), it appears that the spin of the photon field can be written in the alternative form

$$\mathbf{S} = \sum_{s=+,-} \int_{-\infty}^{\infty} \mathbf{g}_s^\dagger(\mathbf{q}; t) \hat{\mathbf{s}}^{\text{proj}} \mathbf{g}_s(\mathbf{q}; t) d^3q. \quad (17.65)$$

Here, $\hat{\mathbf{s}}^{\text{proj}}$ is the so-called projected (superscript: proj) photon spin operator. The i th Cartesian component of this operator is given by

$$\hat{s}_i^{\text{proj}} = (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}) \cdot \mathbf{s}_i \cdot (\mathbf{U} - \hat{\mathbf{q}}\hat{\mathbf{q}}). \quad (17.66)$$

The components of the projected spin operator may be expressed in a much simpler and perhaps surprising form. Hence, by working in Cartesian coordinates it turns out after some algebraic efforts that

$$s_i^{\text{proj}} = \frac{i\hbar}{q^2} q_i \boldsymbol{\Sigma}, \quad (17.67)$$

where q_i is the i th component of the wave vector $\mathbf{q}$. The 3×3 matrix $\boldsymbol{\Sigma}$ is *independent* of the index i , and is given by

$$\boldsymbol{\Sigma} = \begin{pmatrix} 0 & -q_z & q_y \\ q_z & 0 & -q_x \\ -q_y & q_x & 0 \end{pmatrix}. \quad (17.68)$$

With the help of the Levi–Civita tensor $\{\epsilon_{ijk}\}$ the jk th element of this antisymmetric matrix can be written in the form

$$\Sigma_{jk} = - \sum_l \epsilon_{jkl} q_l. \quad (17.69)$$

Due to the fact that the same matrix $\boldsymbol{\Sigma}$ enters all three components of the projected photon spin operator (see (17.67)) these commute mutually, i.e.,

$$\hat{\mathbf{s}}^{\text{proj}} \times \hat{\mathbf{s}}^{\text{proj}} = \mathbf{0} \quad (17.70)$$

in usual vectorial notation.

17.3.4 Eigenvectors and Eigenvalues of the Photon Helicity Operator

To understand the importance of the helicity operator $\hat{h}$, which in the momentum representation is given by $\hat{h} = \hat{\mathbf{s}} \cdot \mathbf{p}/p$ (see (15.112)), we return to the dynamical equations for the complex field vectors $\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t)$ in the wave vector domain (15.70). By making use of the relation in (15.109) (take $\mathbf{a} = \hat{\mathbf{p}} (= \hat{\mathbf{q}})$ and $\mathbf{F} = \boldsymbol{\beta}_{\pm}^{(+)}$) these equations can be written as follows:

$$i\hbar \frac{\partial}{\partial t} \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t) = \pm c_0 q \mathbf{h} \cdot \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t), \quad (17.71)$$

where

$$\mathbf{h} = \frac{1}{p} \sum_i p_i \mathbf{s}_i \quad (17.72)$$

is the matrix representative of the helicity operator, p_i being the i th component of the photon momentum. Before proceeding it is worth emphasizing that the following results also hold in the framework of the photon energy wave function formalism. This is so because $\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t)$ and $\mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t)$ satisfy dynamical form-identical

equations. When the ansatz

$$\boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}; t) = \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}, c_0 q) e^{-i c_0 q t} \quad (17.73)$$

is inserted into the dynamical equations in (17.71) one obtains the following time independent equations

$$\mathbf{h} \cdot \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}, c_0 q) = \pm \hbar \boldsymbol{\beta}_{\pm}^{(+)}(\mathbf{q}, c_0 q). \quad (17.74)$$

The relation in (15.71) finally leads to the matrix equations

$$\mathbf{h} \cdot \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}) = \pm \hbar \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{q}}). \quad (17.75)$$

The equations in (17.75) tell us that the eigenvalues of the photon helicity operator are $+\hbar$ and $-\hbar$, and that the corresponding (normalized) eigenvectors are $\hat{\mathbf{e}}_{+}(\hat{\mathbf{q}})$ and $\hat{\mathbf{e}}_{-}(\hat{\mathbf{q}})$, respectively.

Chapter 18

Photon Emission from Micro- and Mesoscopic Sources: Near-Field Aspects

Until now we have discussed photon wave mechanics in free space only. From an observational point of view it is absolutely necessary however that we extend the fundamental theory so as to take into account the photon–matter interaction. In this interaction, photons are either generated or destroyed. A photon is generated in an emission process from a source and destroyed in an absorption process in a detector. When the source and detector are in each others far-field zones the emission and absorption processes can be studied separately at least in the framework of first quantization, but if the source and detector are in near-field contact the two processes interfere in an extremely complicated manner. In the presence of field–matter interactions, photon wave mechanics is a very broad field of study, and in the present chapter we shall discuss the emission processes only, paying particular attention to the electrodynamics in the rim zone of the source. Even the photon emission process is quite complicated to tackle theoretically, because the photon during the emission process acts back on the source particles and change their dynamics. In the quite limited framework of linear electrodynamics we discussed this back-action on the basis of the coupled-antenna theory in Chap. 13. Although we did not relate the coupled-antenna theory to photon wave mechanics as such this can be done if one wishes so. In this chapter, we shall not address the back-action problem. One may address the photon emission theme starting from the complex field theory (Chap. 15), the energy wave function formalism (Chap. 16), or the four-potential theory (Chap. 16). Rigorous descriptions will result in the same observational predictions in all three schemes of photon wave mechanics. Different approximations made during intermediate calculations in the various formulations may of course lead to *unphysical* differences in the final prediction. In what follows we shall base our analysis mainly on the photon energy wave function theory, and certain modifications of this theory’s near-field aspects. The close resemblance of the energy wave function formalism to the complex field theory makes it easy to “translate” the treatment below to the CF-theory. From a conceptual point of view the near-field aspects of the photon emission process appear formally in a quite different disguise in the four-potential theory, and in the final section of this chapter we shall briefly discuss this formal change in our point of view.

18.1 Microscopic Electrodynamics Based on D - and H -Fields

18.1.1 New Microscopic Field Equations

In Sect. 10.4, the microscopic current density, $\mathbf{J}(\mathbf{r}, t)$, was divided into two parts, and thereby two new vector fields were introduced, namely the generalized polarization, $\mathbf{P}(\mathbf{r}, t)$, and magnetization, $\mathbf{M}(\mathbf{r}, t)$; see (10.41). For a given choice of these vector fields two new microscopic fields $\mathbf{D}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$ then were defined, see (10.47) and (10.48). In the microscopic Maxwell–Lorentz equations, given in (2.1)–(2.4), the primary quantities are on the field side $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$, and on the particle side $\mathbf{J}(\mathbf{r}, t)$ and $\rho(\mathbf{r}, t)$. For what follows in this chapter and later on, it is convenient to replace these equations by new ones involving on the field side $\mathbf{D}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$, and on the particle side $\mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t)$. As we shall realize only a certain combination of these material quantities is needed, basically.

By combining (10.47), (10.48), and (2.1) one obtains after a few rearrangements

$$\nabla \times (\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)) + \frac{\partial}{\partial t} (\mu_0 \mathbf{H}(\mathbf{r}, t)) = -\epsilon_0^{-1} \mathbf{W}(\mathbf{r}, t), \quad (18.1)$$

where

$$\mathbf{W}(\mathbf{r}, t) = \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathbf{M}(\mathbf{r}, t) - \nabla \times \mathbf{P}(\mathbf{r}, t). \quad (18.2)$$

Two comments should be given to these equations: (1) As it will soon become clear, it is useful to consider the scaled quantities $\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)$ and $\mu_0 \mathbf{H}(\mathbf{r}, t)$ as the primary ones when photon wave mechanics is extended to coupled field–matter studies and (2) in contrast to the source free Maxwell–Lorentz equation in (2.1) the new equation has a source term (proportional to) $\mathbf{W}(\mathbf{r}, t)$. When one inserts (10.41), (10.47), and (10.48), written in the appropriate forms, into the Maxwell–Lorentz equation in (2.3), this inhomogeneous field equation is turned into a homogeneous one, viz.,

$$\nabla \times (\mu_0 \mathbf{H}(\mathbf{r}, t)) - \frac{1}{c_0^2} \frac{\partial}{\partial t} (\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)) = \mathbf{0}. \quad (18.3)$$

To rewrite the inhomogeneous Maxwell–Lorentz equation in (2.2) in the desired form one utilizes (10.47) and the relation in (10.44). Thus, one obtains

$$\nabla \cdot (\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)) = 0. \quad (18.4)$$

If $\mathbf{P}(\mathbf{r}, t)$ relates to the total charge density one gets the result of (18.4). If instead $\mathbf{P}(\mathbf{r}, t)$ relates to only a part of the total charge density (ρ^{ext} excluded) one obtains (10.50). With the help of (10.48), and the fact that the longitudinal part of the magnetization vector plays no physical role, so that we may take

$$\mathbf{M}_L(\mathbf{r}, t) = \mathbf{0}, \quad (18.5)$$

the last Maxwell–Lorentz equation (2.4) is transformed into

$$\nabla \cdot (\mu_0 \mathbf{H}(\mathbf{r}, t)) = 0, \quad (18.6)$$

since $\nabla \cdot \mathbf{M} = \nabla \cdot \mathbf{M}_T = 0$.

By now, the original set of Maxwell–Lorentz equations ((2.1)–(2.4)) has been replaced by a set of new microscopic field equations ((18.1), (18.3), (18.4) and (18.6)). The two sets are equivalent from a physical point of view, but the new set allows us to see certain aspects of the near-field photon–matter interaction in a broader perspective, as we soon shall realize. Of the original vector field $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ only the magnetic field is a genuine transverse vector field. In contrast, both of the new fields $\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)$ and $\mu_0 \mathbf{H}(\mathbf{r}, t)$ are transverse vector fields, cf. (18.4) and (18.6). The field $\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)$ is always so, and the field $\mu_0 \mathbf{H}(\mathbf{r}, t)$ is made so by the choice in (18.5). In the original Maxwell–Lorentz formulation of microscopic electrodynamics two of the four field equations are inhomogeneous ((2.2) and (2.3)), and thus involve, via $\mathbf{J}(\mathbf{r}, t)$ and $\rho(\mathbf{r}, t)$, the relevant material properties in a manifest manner. In the new formulation only one field equation is inhomogeneous (18.1), and the field–matter interaction involves only one material vector field, viz. $\mathbf{W}(\mathbf{r}, t)$ (18.2).

18.1.2 Duality Between Old and New Transverse Electrodynamics: New Wave Equations

The analogy between the old and new microscopic field equations becomes deeper if one compares the new equations to the transverse set of Maxwell–Lorentz equations ((9.25), (9.26) and the transversality conditions $\nabla \cdot \mathbf{E}_T(\mathbf{r}, t) = \nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0$). This is not surprising for two reasons: (1) The charge density $\rho(\mathbf{r}, t)$ relates only to the longitudinal part of the electric field, which means that the transverse set of Maxwell–Lorentz equations contains only one material vector field, namely, $\mathbf{J}_T(\mathbf{r}, t)$, and (2) the vector field $\mathbf{W}(\mathbf{r}, t)$ is a genuine transverse vector field, i.e.,

$$\mathbf{W}(\mathbf{r}, t) = \mathbf{W}_T(\mathbf{r}, t), \quad (18.7)$$

since from (18.2) one immediately obtains $\nabla \cdot \mathbf{W}(\mathbf{r}, t) = 0$, remembering that $\nabla \cdot \mathbf{M}(\mathbf{r}, t) = 0$. The following duality

$$\mu_0 \mathbf{H}(\mathbf{r}, t) \Leftrightarrow \mathbf{E}_T(\mathbf{r}, t), \quad (18.8)$$

$$\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t) \Leftrightarrow -c_0^2 \mathbf{B}(\mathbf{r}, t), \quad (18.9)$$

$$\mathbf{W}(\mathbf{r}, t) \Leftrightarrow \mathbf{J}_T(\mathbf{r}, t), \quad (18.10)$$

thus relates the transverse set of Maxwell–Lorentz equations to our new field equations, as the reader may convince himself of by making the above-mentioned (left

to right) replacements in (18.1), (18.3), (18.4), and (18.6). The duality given in the source connection in (18.10) is interesting from a near-field perspective. Thus, the $\mathbf{J}_T$ -source expands over the electronic source domain *plus* the rim zone, in general, but at first sight the reader may be tempted to believe that the $\mathbf{W}_T$ -source has the extension of the electronic domain. As we soon will understand, the new microscopic field equations offer us a broader physical perspective of the photon emission process.

The transverse fields $\mathbf{E}_T(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ satisfy the wave equations in (9.30) and (9.31), the last equation possibly with $\mathbf{J}(\mathbf{r}, t)$ replaced by $\mathbf{J}_T(\mathbf{r}, t)$. From the duality relations in (18.8)–(18.10) it therefore follows that the new transverse field vectors $\epsilon_0^{-1}\mathbf{D}(\mathbf{r}, t)$ and $\mu_0\mathbf{H}(\mathbf{r}, t)$ satisfy the following inhomogeneous wave equations:

$$\square(\epsilon_0^{-1}\mathbf{D}(\mathbf{r}, t)) = \epsilon_0^{-1}\nabla \times \mathbf{W}_T(\mathbf{r}, t), \quad (18.11)$$

$$\square(\mu_0\mathbf{H}(\mathbf{r}, t)) = \mu_0 \frac{\partial}{\partial t} \mathbf{W}_T(\mathbf{r}, t). \quad (18.12)$$

In ending this section, we can conclude that in the new field description the primary fields $\epsilon_0^{-1}\mathbf{D}$ and $\mu_0\mathbf{H}$ always are genuine transverse vector fields, but when the choice of potentials is changed the quantities called fields and sources are modified.

18.2 The Photon Embryo Concept

18.2.1 Dynamical Photon Wave Function Variables

The new formulation of microscopic classical electrodynamics we now apply in photon wave mechanics, and in particular to a study of single-photon emission processes. To emphasize that we are dealing with one-photon problems all field variables are denoted by small letters in the following, and source terms (matter related quantities) are written with calligraphic capital letters. Photon wave mechanics is related to positive-frequency signals, and our starting point hence is the analytical parts of (18.1), (18.3), (18.4) and (18.6), viz.,

$$\nabla \times (\epsilon_0^{-1}\mathbf{d}^{(+)}(\mathbf{r}, t)) + \frac{\partial}{\partial t}(\mu_0\mathbf{h}^{(+)}(\mathbf{r}, t)) = -\epsilon_0^{-1}\mathcal{W}^{(+)}(\mathbf{r}, t), \quad (18.13)$$

$$\nabla \times (\mu_0\mathbf{h}^{(+)}(\mathbf{r}, t)) - \frac{1}{c_0^2} \frac{\partial}{\partial t}(\epsilon_0^{-1}\mathbf{d}^{(+)}(\mathbf{r}, t)) = \mathbf{0}, \quad (18.14)$$

$$\nabla \cdot (\epsilon_0^{-1}\mathbf{d}^{(+)}(\mathbf{r}, t)) = 0, \quad (18.15)$$

$$\nabla \cdot (\mu_0\mathbf{h}^{(+)}(\mathbf{r}, t)) = 0. \quad (18.16)$$

Now, two so-called generalized photon wave function variables $\mathbf{v}_+^{(+)}(\mathbf{r}, t)$ and $\mathbf{v}_-^{(+)}(\mathbf{r}, t)$ are introduced by the definitions

$$\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(\epsilon_0^{-1} \mathbf{d}^{(+)}(\mathbf{r}, t) \pm i c_0 \mu_0 \mathbf{h}^{(+)}(\mathbf{r}, t) \right). \quad (18.17)$$

The variables above are closely related to the positive-frequency Riemann–Silberstein vectors in (16.23). To obtain the relation between $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t)$ and $\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$ we utilize the transversality of the $\mathbf{D}$ -field (18.4). For the analytical photon signals this gives via (10.47)

$$\mathbf{d}^{(+)}(\mathbf{r}, t) = \mathbf{d}_{\text{T}}^{(+)}(\mathbf{r}, t) = \epsilon_0 \mathbf{e}_{\text{T}}^{(+)}(\mathbf{r}, t) + \mathcal{P}_{\text{T}}^{(+)}(\mathbf{r}, t) \quad (18.18)$$

and

$$\mathbf{d}_{\text{L}}^{(+)}(\mathbf{r}, t) = \epsilon_0 \mathbf{e}_{\text{L}}^{(+)}(\mathbf{r}, t) + \mathcal{P}_{\text{L}}^{(+)}(\mathbf{r}, t) = \mathbf{0}. \quad (18.19)$$

By inserting (18.18), and the expression

$$\mathbf{h}^{(+)}(\mathbf{r}, t) = \mu_0^{-1} \mathbf{b}^{(+)}(\mathbf{r}, t) - \mathcal{M}^{(+)}(\mathbf{r}, t), \quad (18.20)$$

where $\mathcal{M}^{(+)}(\mathbf{r}, t) = \mathcal{M}_{\text{T}}^{(+)}(\mathbf{r}, t)$ (cf. (18.5)), into (18.17) one gets

$$\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) + \frac{1}{\sqrt{2\epsilon_0}} \left(\mathcal{P}_{\text{T}}^{(+)}(\mathbf{r}, t) \mp i c_0 \mathcal{M}^{(+)}(\mathbf{r}, t) \right). \quad (18.21)$$

By adding to the right side of (18.21) the null-vector in (18.19) one obtains the alternative forms

$$\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) + \frac{1}{\sqrt{2\epsilon}} \left(\mathcal{P}^{(+)}(\mathbf{r}, t) \mp i c_0 \mathcal{M}^{(+)}(\mathbf{r}, t) \right) + \sqrt{\frac{\epsilon_0}{2}} \mathbf{e}_{\text{L}}^{(+)}(\mathbf{r}, t). \quad (18.22)$$

It appears from the relations in (18.22) that the wave function variables $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t)$ and $\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$ are identical in the far zone of matter. If the terms containing $\mathcal{P}^{(+)}$ and $\mathcal{M}^{(+)}$ for some reason can be neglected one has

$$\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) + \sqrt{\frac{\epsilon_0}{2}} \mathbf{e}_{\text{L}}^{(+)}(\mathbf{r}, t). \quad (18.23)$$

This relation (or (18.22)) shows an important difference between the two wave function variables: The Riemann–Silberstein vectors $\mathbf{f}_{\pm}^{(+)}$ depend, as we know, only on the dynamical variables of the (transverse) electromagnetic field, whereas the generalized vectors $\mathbf{v}_{\pm}^{(+)}$ additionally also depend on the dynamical variables of the particle system, cf. (9.54) e.g.. In empty space, $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$, and the wave mechanics of free photons therefore will be the same whether one base the theory on the original Maxwell–Lorentz equations or on the new microscopic field equations. In wave mechanical studies of photon–matter interactions deviations

between the two formulations only appear in the near-field zone of, and inside, matter. If (18.23) is a good approximation the difference $\mathbf{v}_{\pm}^{(+)} - \mathbf{f}_{\pm}^{(+)}$ is the same for both helicity components.

18.2.2 Dynamical Equations for the Photon Wave Function Variables

Starting from (18.13) and (18.14) the reader may convince himself that the generalized photon wave function variables satisfy the dynamical equations

$$i\hbar \frac{\partial}{\partial t} \mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \hbar \nabla \times \mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) \pm \frac{\hbar c_0}{\sqrt{2\epsilon_0}} \mathcal{W}^{(+)}(\mathbf{r}, t), \quad (18.24)$$

where

$$\mathcal{W}^{(+)}(\mathbf{r}, t) = \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathcal{M}^{(+)}(\mathbf{r}, t) - \nabla \times \mathcal{P}^{(+)}(\mathbf{r}, t). \quad (18.25)$$

In the absence of matter the $\mathbf{v}_{\pm}^{(+)}$'s satisfy the dynamical equations

$$i\hbar \frac{\partial}{\partial t} \mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \hbar \nabla \times \mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) \quad (18.26)$$

since $\mathcal{W}^{(+)}(\mathbf{r}, t) = \mathbf{0}$. In the framework of the photon energy wave function formalism the equations in (18.26) are identical to the Schrödinger-like wave equations for the two helicity species of the photon due to the fact that $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$ in free space; cf. (18.23) (see also (16.24)). Although the *form* of the dynamical equation for each of the $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t)$'s is unique the dynamical photon wave function variables vary according to the choices made for $\mathcal{P}_{\text{T}}^{(+)}(\mathbf{r}, t)$ and $\mathcal{M}_{\text{T}}^{(+)}(\mathbf{r}, t)$. The different choices for the generalized magnetization and transverse polarization are connected in the manner given in (10.45) and (10.46). It should be emphasized that a change of choice not only affects the photon wave function variables but also the source $[\mathcal{W}^{(+)}(\mathbf{r}, t)]$ term. It is not possible however to make a choice which takes one from $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t)$ to $\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t)$. As we know, it is the duality transformation, $\mu_0 \mathbf{h}^{(+)} \Rightarrow \mathbf{e}_{\text{T}}^{(+)}(\mathbf{r}, t)$, $\epsilon_0^{-1} \mathbf{d}^{(+)} \Rightarrow -c_0^2 \mathbf{b}^{(+)}$, $\mathcal{W}^{(+)} \Rightarrow \mathcal{J}_{\text{T}}^{(+)}$, which gives us the dynamical equation for the $\mathbf{f}_{\pm}^{(+)}$'s, viz.,

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = \pm c_0 \hbar \nabla \times \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) - \frac{i\hbar}{\sqrt{2\epsilon_0}} \mathcal{J}_{\text{T}}^{(+)}(\mathbf{r}, t). \quad (18.27)$$

Since the transverse current density is invariant against the transformation given by (10.45) and (10.46), it is obvious that $\mathbf{v}_{\pm}^{(+)}$ cannot be transformed into $\mathbf{f}_{\pm}^{(+)}$ by a transformation of the material fields. This conclusion also follows from the fact that the definition of the $\mathbf{f}_{\pm}^{(+)}$'s does not involve matter properties.

18.2.3 Photon Embryo in Momentum Space

If one applies the Fourier integral transformation

$$V(\mathbf{r}, t) = h^{-3} \int_{-\infty}^{\infty} V(\mathbf{p}; t) e^{i\hat{\mathbf{p}} \cdot \hat{\mathbf{r}} / \hbar} d^3 p \quad (18.28)$$

to $\mathbf{v}_{\pm}^{(+)}(\mathbf{r}, t)$ and $\mathcal{W}^{(+)}(\mathbf{r}, t)$, the dynamical equations in (18.24) can readily be transferred to the momentum representation. Thus,

$$i\hbar \frac{\partial}{\partial t} \mathbf{v}_{\pm}^{(+)}(\mathbf{p}; t) = \pm i c_0 \mathbf{p} \times \mathbf{v}_{\pm}^{(+)}(\mathbf{p}; t) \pm \frac{\hbar c_0}{\sqrt{2\epsilon_0}} \mathcal{W}^{(+)}(\mathbf{p}; t), \quad (18.29)$$

where

$$\mathcal{W}^{(+)}(\mathbf{p}, t) = \frac{1}{c_0^2} \frac{\partial}{\partial t} \mathcal{M}^{(+)}(\mathbf{p}; t) - \frac{i}{\hbar} \mathbf{p} \times \mathcal{P}^{(+)}(\mathbf{p}; t). \quad (18.30)$$

In order to solve the dynamical equations in (18.29) for a prescribed $\mathcal{W}^{(+)}(\mathbf{p}; t)$, one introduces scalar amplitudes through the ansatz's

$$\mathbf{v}_{\pm}^{(+)}(\mathbf{p}; t) = v_{\pm}^{(+)}(\mathbf{p}; t) \hat{\mathbf{e}}_{\pm}(\hat{\mathbf{p}}), \quad (18.31)$$

and resolves the transverse source field $\mathcal{W}^{(+)}(\mathbf{p}; t) = \mathcal{W}_{\mathbf{T}}^{(+)}(\mathbf{p}; t)$ into its two helicity components, i.e.,

$$\mathcal{W}^{(+)}(\mathbf{p}; t) = \mathcal{W}_{+}^{(+)}(\mathbf{p}; t) \hat{\mathbf{e}}_{+}(\hat{\mathbf{p}}) + \mathcal{W}_{-}^{(+)}(\mathbf{p}; t) \hat{\mathbf{e}}_{-}(\hat{\mathbf{p}}), \quad (18.32)$$

where

$$\mathcal{W}_{\pm}^{(+)}(\mathbf{p}; t) = \hat{\mathbf{e}}_{\pm}^{*}(\hat{\mathbf{p}}) \cdot \mathcal{W}^{(+)}(\mathbf{p}; t). \quad (18.33)$$

The ansatz's in (18.31) are analogous to the one's used in (15.71) to transform (15.70) into (15.73), and the decomposition given by (18.32) and (18.33) follows from the dyadic relation in (15.57), remembering that $\mathcal{W}^{(+)}(\mathbf{p}; t)$ is orthogonal to $\hat{\mathbf{p}} = \hat{\mathbf{q}}$. In the same manner as (15.73) is obtained from (15.70), we here are led from (18.29) to the following dynamical equations for the scalar functions $v_{\pm}^{(+)}(\mathbf{p}; t)$:

$$i\hbar \frac{\partial}{\partial t} v_{\pm}^{(+)}(\mathbf{p}; t) = c_0 p v_{\pm}^{(+)}(\mathbf{p}; t) \pm \frac{\hbar c_0}{\sqrt{2\epsilon_0}} \mathcal{W}_{\pm}^{(+)}(\mathbf{p}; t). \quad (18.34)$$

Let us now assume that the source term vanishes in the remote past that is

$$\mathcal{W}_{\pm}^{(+)}(\mathbf{p}; t \rightarrow -\infty) = 0. \quad (18.35)$$

With this boundary condition the two solutions to (18.34) are given by

$$v_{\pm}^{(+)}(\mathbf{p}; t) = \mp \frac{ic_0}{\sqrt{2\epsilon_0}} e^{-ic_0 p t / \hbar} \int_{-\infty}^t \mathcal{W}_{\pm}^{(+)}(\mathbf{p}; t') e^{ic_0 p t' / \hbar} dt'. \quad (18.36)$$

Together, (18.30)–(18.33) and (18.36) describe, for the given choice of potentials, the photon wave mechanical emission process in the momentum–time domain. If the single-photon Riemann–Silberstein vectors $\mathbf{f}_{\pm}^{(+)}$ are used in a characterization of the emission process it appears upon a comparison of the dynamical equations in (18.24) and (18.27) that the scalar amplitudes $f_{\pm}^{(+)}(\mathbf{p}; t)$ must be given by

$$f_{\pm}^{(+)}(\mathbf{p}; t) = -\frac{1}{\sqrt{2\epsilon_0}} e^{-ic_0 p t / \hbar} \int_{-\infty}^t \mathcal{J}_T^{(+)}(\mathbf{p}; t') e^{ic_0 p t' / \hbar} dt', \quad (18.37)$$

provided of course that the transverse source current density vanishes in the remote part, i.e.,

$$\mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}; t \rightarrow -\infty) = 0. \quad (18.38)$$

The quantities

$$\mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}; t) = \hat{\mathbf{e}}_{\pm}^* \cdot \mathcal{J}_T^{(+)}(\mathbf{p}; t) \quad (18.39)$$

denote, as the reader may already have guessed, the two helicity components of the transverse current density. The results in (18.36) and (18.37), together with the relevant extra expressions, describe what we may call various photon embryo states. These states are not uniquely defined due to the fact that a genuine photon wave function concept can only be introduced in free space. In a photon emission (or absorption) process, only the properties of the coupled photon–particle system can be given a precise physical meaning.

It is of interest to indicate how a given photon embryo evolves into the free photon wave function. We shall exemplify this below starting from the Riemann–Silberstein expressions in (18.37). In order to make contact to the description in Sect. 16.1.3, we characterize the photon emission process using spinor notation. The six-component object

$$\Psi(\mathbf{p}; t) = \begin{pmatrix} g_+(\mathbf{p}; t) \hat{\mathbf{e}}_+(\hat{\mathbf{p}}) \\ g_-(\mathbf{p}; t) \hat{\mathbf{e}}_-(\hat{\mathbf{p}}) \end{pmatrix} \equiv h^{-3/2} (c_0 p)^{-1/2} \begin{pmatrix} f_+^{(+)}(\mathbf{p}; t) \hat{\mathbf{e}}_+(\hat{\mathbf{p}}) \\ f_-^{(+)}(\mathbf{p}; t) \hat{\mathbf{e}}_-(\hat{\mathbf{p}}) \end{pmatrix} \quad (18.40)$$

thus enables us to calculate the energy of the photon embryo at the time $t = t$ via the formula

$$E(t) = \int_{-\infty}^{\infty} c_0 p \Psi^\dagger(\mathbf{p}; t) \cdot \Psi(\mathbf{p}; t) d^3 p. \quad (18.41)$$

As indicated, the energy $E(t)$ of the embryo is not conserved in time. In the limit $t \rightarrow \infty$ the photon has for sure been created in the emission process, and the wave function of the emerged photon hence is given by

$$\Phi(\mathbf{p}; t) = \lim_{t \rightarrow \infty} \Psi(\mathbf{p}; t). \quad (18.42)$$

The upper and lower components of the wave function of the created photon (16.47) both have the time dependence $\exp(-i c_0 p t / \hbar)$; see (16.45).

18.3 One-Photon Sources

How one can obtain a guarantee that precisely one photon emerges from the emission process? Since the photon emission process is completely controlled by the (selfconsistently determined) current density of the source one may as well ask the following question: What kind of constraint must one impose on a given source current density distribution to ensure that just one photon emerges from the emission process in the wave mechanical description? In this section, we shall answer this question working in the momentum representation.

A one-photon state is normalized provided the condition in (16.48) is satisfied. The wave function of the born photon, $\Phi(\mathbf{p}; t)$, can be related to the source current density by means of the asymptotic connection in (18.42). In basing the calculations on $\Psi(\mathbf{p}; t)$ one necessarily from the outset works with the Riemann–Silberstein photon wave functions $f_{\pm}^{(+)}(\mathbf{p}; t)$; see (18.40). One would reach the same conclusion concerning the condition for having a one-photon source if one had started from the generalized photon wave function variables $v_{\pm}^{(+)}(\mathbf{p}; t)$ because

$$\lim_{t \rightarrow \infty} v_{\pm}^{(+)}(\mathbf{p}; t) = \lim_{t \rightarrow \infty} f_{\pm}^{(+)}(\mathbf{p}; t). \quad (18.43)$$

That this is so is indirectly also obvious from the fact that observational effects cannot depend on the choice made for the polarization and magnetization potentials. In the limit $t \rightarrow \infty$ one obtains from (18.37)

$$f_{\pm}^{(+)}(\mathbf{p}; t \rightarrow \infty) = -\frac{1}{\sqrt{2\epsilon_0}} \mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) \exp^{-i c_0 p t / \hbar}, \quad (18.44)$$

where

$$\mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) = \int_{-\infty}^{\infty} \mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}; t) e^{i c_0 p t / \hbar} dt \quad (18.45)$$

are the momentum–frequency transforms of $\mathcal{J}_{T,\pm}^{(+)}(\mathbf{r}; t)$. Asymptotically, the *scaled* scalar energy wave functions for the two helicity states hence are given by

$$g_{\pm}(\mathbf{p}; t \rightarrow \infty) = -h^{-3/2} (2\epsilon_0 c_0 p)^{-1/2} \mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) \exp^{-i c_0 p t / \hbar}; \quad (18.46)$$

cf. (18.40). The result here has precisely the free photon form given in (16.45), and the wave function amplitudes are

$$g_{\pm}(\mathbf{p}) = -h^{-3/2}(2\epsilon_0 c_0 p)^{-1/2} \mathcal{J}_{T,\pm}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}). \quad (18.47)$$

The normalization condition for the one-photon state, viz.,

$$\sum_{s=+,-} \int_{-\infty}^{\infty} |g_s(\mathbf{p})|^2 d^3 p = 1, \quad (18.48)$$

now may be expressed in terms of the momentum–frequency transforms of the transverse source current densities' helicity components as follows:

$$\frac{1}{2h^3 \epsilon_0 c_0} \sum_{s=+,-} \int_{-\infty}^{\infty} \frac{1}{p} |\mathcal{J}_{T,s}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar})|^2 d^3 p = 1. \quad (18.49)$$

The orthogonality of the two helicity states, expressed by (15.56), allows one to write the normalization condition directly in terms of the integral of the vectorial quantity

$$\mathcal{J}_T^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) = \sum_{s=+,-} \mathcal{J}_{T,s}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) \hat{\mathbf{e}}_s(\hat{\mathbf{p}}) \quad (18.50)$$

over momentum space. Thus, one obtains

$$\frac{1}{2h^3 \epsilon_0 c_0} \int_{-\infty}^{\infty} \frac{1}{p} \left[\mathcal{J}_T^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) \right]^* \cdot \mathcal{J}_T^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) d^3 p = 1. \quad (18.51)$$

In most applications, one would prescribe or calculate the source current density itself, i.e., $\mathbf{J}(\mathbf{r}, t)$, or its double Fourier transform $\mathbf{J}(\mathbf{p}, c_0 p/\hbar)$, and not the analytical part of the transverse current density. A knowledge of $\mathbf{J}(\mathbf{p}, c_0 p/\hbar)$ immediately gives us its analytical part, viz., $\mathbf{J}^{(+)}(\mathbf{p}, c_0 p/\hbar) = \mathbf{J}(\mathbf{p}, c_0 p/\hbar > 0)$. It is not difficult to set up the one-photon normalization condition in terms of the positive-frequency part of the current density itself. Since the transverse delta function, given in momentum space by $\delta_T(\hat{\mathbf{p}}) = U - \hat{\mathbf{p}}\hat{\mathbf{p}}$, is real and satisfies the relation

$$\delta_T(\hat{\mathbf{p}}) = \delta_T(\hat{\mathbf{p}}) \cdot \delta_T(\hat{\mathbf{p}}), \quad (18.52)$$

it is realized that the normalization condition also can be written in the integral form

$$\frac{1}{2h^3 \epsilon_0 c_0} \int_{-\infty}^{\infty} \frac{1}{p} \left[\mathcal{J}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) \right]^* \cdot (U - \hat{\mathbf{p}}\hat{\mathbf{p}}) \cdot \mathcal{J}^{(+)}(\mathbf{p}, \frac{c_0 p}{\hbar}) d^3 p = 1. \quad (18.53)$$

Starting from a given source current density $\mathbf{J}(\mathbf{p}, c_0 p/\hbar)$ one adjusts the magnitude of its amplitude until the new current density $\mathcal{J}(\mathbf{p}, c_0 p/\hbar > 0)$ satisfies (18.53). This adjustment guarantees that precisely one photon emerges in the emission process. Later on when we briefly discuss wave-packet and wave-train photons use will be made of (18.53).

18.4 Propagator Description of Photon Embryo in Space–Time

18.4.1 Remarks on the Classical Source Term $W(\mathbf{r}, t)$

In Sect. 18.1, it was realized that if one bases microscopic classical electrodynamics on $\mathbf{D}$ - and $\mathbf{H}$ -fields the source term in the set of dynamical field equations is the vector field $\mathbf{W}(\mathbf{r}, t)$, given in terms of the generalized magnetization and polarization in (18.2). Without loss of generality one can assume that the source term is a genuine transverse vector field, $\mathbf{W}(\mathbf{r}, t) = \mathbf{W}_T(\mathbf{r}, t)$; cf. the considerations leading to (18.7). In Sect. 10.4.1, the $\mathbf{P}(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t)$ vector fields were introduced in such a manner that the combination of the first-order space and time derivatives given in (10.41) equals the invariant microscopic particle current density $\mathbf{J}(\mathbf{r}, t)$. The source field $\mathbf{W}(\mathbf{r}, t)$ is not in general invariant against the transformation of $\mathbf{P}_T(\mathbf{r}, t)$ and $\mathbf{M}(\mathbf{r}, t) = \mathbf{M}_T(\mathbf{r}, t)$ given in (10.45) and (10.46). Since $\nabla \cdot \mathbf{N}_T(\mathbf{r}, t) = 0$ and $\nabla \times \mathbf{P}(\mathbf{r}, t) = \nabla \times \mathbf{P}_T(\mathbf{r}, t)$ the source field is transformed as follows:

$$\mathbf{W}(\mathbf{r}, t) \Rightarrow \mathbf{W}'(\mathbf{r}, t) = \mathbf{W}(\mathbf{r}, t) - \square \mathbf{N}_T(\mathbf{r}, t). \quad (18.54)$$

Hence, only if $\mathbf{N}_T(\mathbf{r}, t)$ satisfies the wave equation $\square \mathbf{N}_T(\mathbf{r}, t) = 0$ will $\mathbf{W}(\mathbf{r}, t)$ be an invariant quantity.

What can be said about the spatial extension of $\mathbf{W}(\mathbf{r}, t)$? The combination of $\mathbf{P}_T(\mathbf{r}, t)$ and $\mathbf{M}_T(\mathbf{r}, t) = \mathbf{M}(\mathbf{r}, t)$ given in (10.43) has the extension of the rim zone, and there is no reason to expect that the combination of these two quantities which enters the expression for $\mathbf{W}(\mathbf{r}, t)$ (18.2) has a different extension. In general, each of the terms on the right side of (18.2) will extend over the entire rim zone. Since $\mathbf{P}_T(\mathbf{r}, t)$ is nonvanishing in the rim zone so will $\nabla \times \mathbf{P}_T(\mathbf{r}, t)$ be, in general. In the transformation of $\mathbf{P}_T(\mathbf{r}, t)$ (10.45), the involved $\mathbf{N}_T(\mathbf{r}, t)$ -field thus also extends over the entire rim zone. In consequence, the transformation of the generalized magnetization given by (10.46) tells us that also $\mathbf{M}(\mathbf{r}, t)$ is nonvanishing in the near-field domain.

18.4.2 Propagator Solutions of the Wave Equations for $\mathbf{D}(\mathbf{r}, t)$ and $\mathbf{H}(\mathbf{r}, t)$

We know from previous analyses in this book that the solution of the inhomogeneous wave equation for the transverse electric field (9.30) can be expressed in terms of the scalar propagator in the form given in (10.4). By a comparison of (18.11) and (18.12) to (9.30) the following propagator solutions are readily obtained for $\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)$ and $\mu_0 \mathbf{H}(\mathbf{r}, t)$:

$$\epsilon_0^{-1} \mathbf{D}(\mathbf{r}, t) = \epsilon_0^{-1} \mathbf{D}^{\text{ext}}(\mathbf{r}, t) - \epsilon_0^{-1} \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \nabla' \times \mathbf{W}(\mathbf{r}', t') d^3 r' dt', \quad (18.55)$$

$$\mu_0 \mathbf{H}(\mathbf{r}, t) = \mu_0 \mathbf{H}^{\text{ext}}(\mathbf{r}, t) - \mu_0 \int_{-\infty}^{\infty} g(|\mathbf{r} - \mathbf{r}'|, t - t') \frac{\partial}{\partial t'} \mathbf{W}(\mathbf{r}', t') d^3 r' dt'. \quad (18.56)$$

It is possible to recover the result in (10.4) from (18.55). We know from the analysis in Sect. 10.4.1 that it is possible to make the choice $\mathbf{P}_T(\mathbf{r}, t) = \mathbf{0}$. For this choice, one has $\epsilon_0^{-1} \mathbf{D} = \mathbf{E}_T$, $\mathbf{W} = c_0^{-2} \partial \mathbf{M} / \partial t$ and $\mathbf{J}_T = \nabla \times \mathbf{M}$. From the last two relations one gets $\epsilon_0^{-1} c_0^{-2} \partial (\nabla \times \mathbf{M}) / \partial t = \mu_0 \partial \mathbf{J}_T / \partial t$. The choice $\mathbf{P}_T = \mathbf{0}$ therefore leads from (18.55) to (10.4). The reader may verify to himself that the same choice transforms (18.12) into

$$\square \mathbf{B}(\mathbf{r}, t) = \mu_0 \nabla^2 \mathbf{M}(\mathbf{r}, t), \quad (18.57)$$

and since $\nabla \times \mathbf{J}_T = \nabla \times (\nabla \times \mathbf{M}) = -\nabla^2 \mathbf{M}$, (18.57) is just the space–time version of the wave equation in (3.50).

18.4.3 Propagation of Embryo State

On the basis of the results in (18.55) and (18.56) propagator expressions relating the generalized photon wave function variables $v_{\pm}^{(+)}(\mathbf{r}, t)$ to the near-field source strength $\mathbf{W}^{(+)}(\mathbf{r}, t)$ can now be obtained. The relevant quantities for the one-photon emission process hence are

$$\epsilon_0^{-1} \mathbf{d}^{(+)}(\mathbf{r}, t) = -\epsilon_0^{-1} \int_{-\infty}^{\infty} g(R, \tau) \nabla' \times \mathbf{W}^{(+)}(\mathbf{r}', t') d^3 r' dt', \quad (18.58)$$

and

$$\mu_0 \mathbf{h}^{(+)}(\mathbf{r}, t) = -\mu_0 \int_{-\infty}^{\infty} g(R, \tau) \frac{\partial}{\partial t'} \mathbf{W}^{(+)}(\mathbf{r}', t') d^3 r' dt', \quad (18.59)$$

with the usual abbreviations $|\mathbf{r} - \mathbf{r}'| = R$ and $t - t' = \tau$. By inserting the expressions above into (18.17) one obtains in compact notation

$$v_{\pm}^{(+)}(\mathbf{r}, t) = -\frac{1}{\sqrt{2\epsilon_0}} \int_{-\infty}^{\infty} g(R, \tau) \left[\pm \frac{i}{c_0} \frac{\partial}{\partial t'} + \nabla' \times \right] \mathbf{W}^{(+)}(\mathbf{r}', t') d^3 r' dt'. \quad (18.60)$$

The photon embryo spinor

$$\boldsymbol{\Psi}(\mathbf{r}, t) \equiv \begin{pmatrix} v_{+}^{(+)} \\ v_{-}^{(+)} \end{pmatrix} \quad (18.61)$$

involves into the free photon wave function $\boldsymbol{\Phi}(\mathbf{r}, t)$ asymptotically assuming that $\mathbf{W}(\mathbf{r}, t')$ vanishes identically for $t' > t_0$, say.

18.5 Gauge and Near-Field Photon Embryos

18.5.1 Dynamical Equations for G- and NF-Photon Variables

In the presence of an electrodynamically active source, the longitudinal part of the electric field is no longer identically zero, and in Sect. 16.3.4 it was shown that the analytical scalar field

$$e_L^{(+)}(\mathbf{q}; t) \equiv \hat{\mathbf{q}} \cdot \mathbf{e}_L^{(+)}(\mathbf{q}; t) \quad (18.62)$$

relates to the dynamical variables of the longitudinal and scalar photons, $a_L^{(+)}(\mathbf{q}; t)$ and $a_0^{(+)}(\mathbf{q}; t)$, in the manner given in (16.102). These variables can be expressed as linear combinations of the gauge and near-field photon variables, $a_G^{(+)}(\mathbf{q}; t)$ and $a_{NF}^{(+)}(\mathbf{q}; t)$, viz.,

$$a_L^{(+)}(\mathbf{q}; t) = \frac{1}{\sqrt{2}} \left(a_G^{(+)}(\mathbf{q}; t) - i a_{NF}^{(+)}(\mathbf{q}; t) \right), \quad (18.63)$$

$$a_0^{(+)}(\mathbf{q}; t) = \frac{1}{\sqrt{2}} \left(a_G^{(+)}(\mathbf{q}; t) + i a_{NF}^{(+)}(\mathbf{q}; t) \right), \quad (18.64)$$

as the reader may verify by inversion of the transformation given in (16.123) and (16.124). By inserting (18.63) and (18.64) into (16.102) the following expression for $e_L^{(+)}(\mathbf{q}; t)$ is obtained:

$$e_L^{(+)}(\mathbf{q}; t) = \frac{1}{\sqrt{2}} \left(c_0 q + i \frac{\partial}{\partial t} \right) a_{NF}^{(+)}(\mathbf{q}; t) - \frac{i}{\sqrt{2}} \left(c_0 q - i \frac{\partial}{\partial t} \right) a_G^{(+)}(\mathbf{q}; t). \quad (18.65)$$

In (18.65), both the G- and NF-variables are needed to calculate the longitudinal electric field. We know however that these dynamical variables are coupled via the Lorenz gauge condition (16.138), and it is therefore possible to calculate $e_L^{(+)}(\mathbf{q}; t)$ from a knowledge of just one of the variables. Thus, one obtains immediately the dynamical equations

$$e_L^{(+)}(\mathbf{q}; t) = \sqrt{2} \left(i \frac{\partial}{\partial t} + c_0 q \right) a_{NF}^{(+)}(\mathbf{q}; t), \quad (18.66)$$

and

$$e_L^{(+)}(\mathbf{q}; t) = i \sqrt{2} \left(i \frac{\partial}{\partial t} - c_0 q \right) a_G^{(+)}(\mathbf{q}; t). \quad (18.67)$$

The analytical part of the one-photon Maxwell–Lorentz equation in (9.37), viz.,

$$i \epsilon_0 e_L^{(+)}(\mathbf{q}; t) = \rho^{(+)}(\mathbf{q}; t), \quad (18.68)$$

allows one to eliminate $e_L^{(+)}$ in the dynamical equations in favour of the source charge density $\rho^{(+)}(\mathbf{q}; t)$. Instead of $\rho^{(+)}(\mathbf{q}; t)$, one may also use the analytical part of the $\mu = 0$ component of the contravariant current density four-vector

$$\{J^\mu\} = (J_0, \mathbf{J}), \quad (18.69)$$

where $J_0 = c_0\rho$. If, as already implied by (18.68), $\rho^{(+)}(\mathbf{q}; t)$ denotes the analytical charge density associated with the one-photon current density $\mathcal{J}^{(+)}$ (given by (18.53)) one has

$$e_L^{(+)}(\mathbf{q}; t) = (i\epsilon_0)^{-1}\rho^{(+)}(\mathbf{q}; t) = (i\epsilon_0 c_0)^{-1}\mathcal{J}_0^{(+)}(\mathbf{q}; t). \quad (18.70)$$

By means of (18.70) the dynamical equations for the gauge and near-field photon variables may finally be written in the following forms:

$$i\hbar \frac{\partial}{\partial t} a_G^{(+)}(\mathbf{q}; t) = c_0 \hbar q a_G^{(+)}(\mathbf{q}; t) - \frac{1}{\epsilon_0 \sqrt{2}} \frac{\hbar}{c_0 q} \mathcal{J}_0^{(+)}(\mathbf{q}; t), \quad (18.71)$$

$$i\hbar \frac{\partial}{\partial t} a_{\text{NF}}^{(+)}(\mathbf{q}; t) = -c_0 \hbar q a_{\text{NF}}^{(+)}(\mathbf{q}; t) + \frac{1}{i\epsilon_0 \sqrt{2}} \frac{\hbar}{c_0 q} \mathcal{J}_0^{(+)}(\mathbf{q}; t). \quad (18.72)$$

In free space, the dynamical equation for the gauge photon variable reduces to the quantum mechanical wave equation for the G-photon (16.126). The dynamical equation for the near-field photon variable, *written in the form given in (18.72)*, does *not* reduce to the Schrödinger-like equation for the free [$\mathcal{J}_0^{(+)}(\mathbf{q}; t) = 0$] near-field photon (16.125); the signs in front of the Hamilton operator $c_0 \hbar q$ are different. It is possible, however, to change the minus sign in (18.72) to a plus sign provided one also changes the form of the inhomogeneous term in (18.72). Thus, it can be shown [177] that the near-field photon variable satisfies the dynamical equation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} a_{\text{NF}}^{(+)}(\mathbf{q}; t) &= c_0 \hbar q a_{\text{NF}}^{(+)}(\mathbf{q}; t) \\ &+ \frac{\hbar}{\epsilon_0 \sqrt{2}} e^{i q c_0 t} \int_{-\infty}^t e^{-i q c_0 t'} \left[\mathcal{J}_0^{(+)}(\mathbf{q}; t') - \mathcal{J}_L^{(+)}(\mathbf{q}; t') \right] dt'. \end{aligned} \quad (18.73)$$

The source term now involves both the charge density and the longitudinal part of the current density in the form of a certain integral over time of their difference (in four-current notation). This much more complicated form of the dynamical equation for the NF-photon variable is the price one has to pay in order to obtain the Schrödinger-like wave equation in (16.125) in the free-space limit.

18.5.2 Time Reversal: Solution of the Dynamical Equations for the G- and NF-Variables

It is interesting to notice that the “wrong” sign on the Hamilton operator in (18.72) also can be removed by time reversal. With the replacement $t \Rightarrow -t$ one thus obtains a dynamical equation

$$i\hbar \frac{\partial}{\partial t} a_{\text{NF}}^{(+)}(\mathbf{q}; -t) = c_0 \hbar q a_{\text{NF}}^{(+)}(\mathbf{q}; -t) - \frac{1}{i\epsilon_0 \sqrt{2}} \frac{\hbar}{c_0 q} \mathcal{J}_0^{(+)}(\mathbf{q}; -t). \quad (18.74)$$

The evolution of the dynamical near-field variable backwards in time asymptotically therefore leads to a Schrödinger-like equation for the free photon wave function $a_{\text{NF}}^{(+)}(\mathbf{q}; -t)$.

We know from the analysis in Sect. 16.4.3 that a near-field photon cannot exist in free space. To fulfil the asymptotic requirement $a_{\text{NF}}^{(+)}(\mathbf{q}; t) \rightarrow \infty = 0$ for the emission process, the solution to the dynamical equation in (18.72) therefore must be

$$a_{\text{NF}}^{(+)}(\mathbf{q}; t) = -\frac{1}{\epsilon_0 \sqrt{2}} \frac{1}{c_0 q} e^{ic_0 q t} \int_{-\infty}^t \mathcal{J}_0^{(+)}(\mathbf{q}; t') e^{-ic_0 q t'} dt'. \quad (18.75)$$

The correctness of this formula follows from the fact that

$$\int_{-\infty}^{\infty} \mathcal{J}_0^{(+)}(\mathbf{q}; t') e^{-ic_0 q t'} dt' = \mathcal{J}_0^{(+)}(\mathbf{q}; -qc_0) = 0, \quad (18.76)$$

since no negative frequencies $\omega = -qc_0$ appear in an analytical signal per definition. The particular solution

$$a_{\text{G}}^{(+)}(\mathbf{q}; t) = \frac{i}{\epsilon_0 \sqrt{2}} \frac{1}{c_0 q} e^{-ic_0 q t} \int_{\infty}^t \mathcal{J}_0^{(+)}(\mathbf{q}; t') e^{ic_0 q t'} dt' \quad (18.77)$$

for the gauge photon variable connects to the situation where the free gauge photon has been eliminated by a suitable gauge transformation within the Lorenz gauge. The, thus, required asymptotic condition on the photon emission process, namely $a_{\text{G}}^{(+)}(\mathbf{q}; t \rightarrow \infty) = 0$ readily is seen to be satisfied by the solution in (18.77).

Chapter 19

Eikonal Theory for Transverse Photons and Massive Particles of Zero Spin

A theory that agrees with another in all predictions within the latter's domain of validity is sometimes called a covering theory. Thus, the microscopic theory of classical electrodynamics based on the Maxwell–Lorentz equations is the covering theory of macroscopic Maxwell electrodynamics which in itself is the covering theory of geometrical optics. The last-mentioned branch of optics deals with phenomena for which the finiteness of the wavelength of light can be neglected. In this approximation, the optical laws may be formulated in the language of geometry, and the basic quantity here is the eikonal, $S(\mathbf{r}; \omega)$. The gradient of the eikonal satisfies the so-called eikonal equation, and the surfaces of constant S are called the geometrical wave surfaces (or wave fronts). The cycle-averaged Poynting vector, which in the mean describes the electromagnetic energy density flow, everywhere in space is in the direction of the normal to the wave surfaces. In geometrical optics, the field energy hence is transported along certain curves, the light rays.

In the present chapter, we shall study some aspects of geometrical optics from the point of view of photon wave mechanics. The wave mechanical theory of the photon originates as we know in a reinterpretation of the microscopic Maxwell–Lorentz equations, and is as such not a covering theory of microscopic classical electrodynamics. Since at short wavelengths the particle aspect of the photon tends to dominate one might expect that the photon probability distribution flows along the light rays in the limit of geometrical optics. We shall verify that this is true, and also realize that the transverse photons attain an effective mass in the high-frequency limit.

The eikonal equation in optics turns out to be form-identical to the Hamilton–Jacobi equation for Hamilton's characteristic function for a single classical particle. As mentioned in the introductory chapter to Part II of this book, this analogy played an important role for de Broglie and Schrödinger in their struggles to unify Newtonian mechanics and the old quantum theory of Planck, Einstein, and Bohr in a more comprehensive theory which better could account for the wealth of new observations being reported. In the last part of the chapter we shall briefly discuss the nonrelativistic Hamilton–Jacobi theory, and its extension to relativistic particles of zero spin.

19.1 Foundations of Geometrical Optics

19.1.1 Macroscopic Maxwell Equations

As a forerunner to the study of the eikonal theory for photons we briefly discuss the foundation of geometrical optics. When the wavelength of the electromagnetic field is very short compared to the length which characterizes the variation of the material properties in a macroscopic system one may in a good first approximation completely neglect the finiteness of the wavelength. The branch of macroscopic electrodynamics which is characterized by such a neglect is, as already said, known as geometrical optics, since the basic laws in the short wavelength limit may be formulated in the language of geometry. The basic equation in geometrical optics is the so-called eikonal equation. The term eikonal comes from the Greek word for image ($\epsilon\iota\kappa\tilde{\omega}\nu$).

To derive the eikonal equation one starts from the macroscopic Maxwell equations in the space–frequency domain, i.e.,

$$\nabla \times \mathbf{E}(\mathbf{r}; \omega) = i\omega \mathbf{B}(\mathbf{r}; \omega), \quad (19.1)$$

$$\nabla \times \mathbf{H}(\mathbf{r}; \omega) = \mathbf{J}(\mathbf{r}; \omega) - i\omega \mathbf{D}(\mathbf{r}; \omega), \quad (19.2)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}; \omega) = \rho(\mathbf{r}; \omega), \quad (19.3)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}; \omega) = 0. \quad (19.4)$$

Although the various macroscopic quantities appearing in these equations here have been denoted by the same symbols as the corresponding microscopic quantities it must be remembered that the macroscopic quantities result from local averaging of the microscopic entities. The macroscopic $\mathbf{D}$ - and $\mathbf{H}$ -fields are defined by

$$\mathbf{D}(\mathbf{r}; \omega) = \epsilon_0 \mathbf{E}(\mathbf{r}; \omega) + \mathbf{P}(\mathbf{r}; \omega), \quad (19.5)$$

and

$$\mathbf{H}(\mathbf{r}; \omega) = \mu_0^{-1} \mathbf{B}(\mathbf{r}; \omega) - \mathbf{M}(\mathbf{r}; \omega), \quad (19.6)$$

where $\mathbf{P}(\mathbf{r}; \omega)$ and $\mathbf{M}(\mathbf{r}; \omega)$ are the (macroscopically defined) electric and magnetic dipole polarizations, respectively. Since $\mathbf{P}(\mathbf{r}; \omega)$ and $\mathbf{M}(\mathbf{r}; \omega)$ here refer to the bound charges, $\mathbf{J}(\mathbf{r}; \omega)$ and $\rho(\mathbf{r}; \omega)$ are the (macroscopically defined) current and charge densities of the free charges. In order to close the theory of macroscopic electrodynamics, the Maxwell equations in (19.1)–(19.4) must be supplemented by a set of material equations (constitutive relations). For the present purpose it is sufficient here to take these in the simple and well known form

$$\mathbf{D}(\mathbf{r}; \omega) = \epsilon_0 \epsilon(\mathbf{r}; \omega) \mathbf{E}(\mathbf{r}; \omega), \quad (19.7)$$

$$\mathbf{B}(\mathbf{r}; \omega) = \mu_0 \mu(\mathbf{r}; \omega) \mathbf{H}(\mathbf{r}; \omega), \quad (19.8)$$

$$\mathbf{J}(\mathbf{r}; \omega) = \sigma(\mathbf{r}; \omega) \mathbf{E}(\mathbf{r}; \omega). \quad (19.9)$$

Nonlocal effects are neglected in these equations because the various vector fields are connected by point relations. The matter response is characterized electro-dynamically by the relative dielectric permittivity (or constant), $\epsilon(\mathbf{r}; \omega)$, the magnetic permeability, $\mu(\mathbf{r}; \omega)$, and by the (specific) conductivity, $\sigma(\mathbf{r}; \omega)$. The three quantities are, as indicated, allowed to depend on position ($\mathbf{r}$), which physically means that the material in question may be inhomogeneous. It is assumed, however, that the matter system is isotropic, since the response functions in (19.7)–(19.9) are taken as scalar quantities. Nonlinear electrodynamic phenomena are neglected on the assumption that the response functions are field independent.

By taking the divergence on both sides of (19.2) one obtains

$$\nabla \cdot \left(\mathbf{D}(\mathbf{r}; \omega) + \frac{i}{\omega} \mathbf{J}(\mathbf{r}; \omega) \right) = 0, \quad (19.10)$$

and from this equation and (19.3) follows the macroscopic equation of continuity for the free charge, viz.,

$$\nabla \cdot \mathbf{J}(\mathbf{r}; \omega) = i\omega\rho(\mathbf{r}; \omega). \quad (19.11)$$

The material relations in (19.7)–(19.9) enable us to eliminate $\mathbf{B}(\mathbf{r}; \omega)$, $\mathbf{D}(\mathbf{r}; \omega)$ and $\mathbf{J}(\mathbf{r}; \omega)$ from (19.1), (19.2), (19.4), and (19.10). As the reader readily may show we thereby obtain the following form of the macroscopic Maxwell equations in the space–frequency domain:

$$\nabla \times \mathbf{E}(\mathbf{r}; \omega) = i\mu_0\omega\mu(\mathbf{r}; \omega)\mathbf{H}(\mathbf{r}; \omega), \quad (19.12)$$

$$\nabla \times \mathbf{H}(\mathbf{r}; \omega) = -i\epsilon_0\omega\epsilon^C(\mathbf{r}; \omega)\mathbf{E}(\mathbf{r}; \omega), \quad (19.13)$$

$$\nabla \cdot (\epsilon^C(\mathbf{r}; \omega)\mathbf{E}(\mathbf{r}; \omega)) = 0, \quad (19.14)$$

$$\nabla \cdot (\mu(\mathbf{r}; \omega)\mathbf{H}(\mathbf{r}; \omega)) = 0, \quad (19.15)$$

where

$$\epsilon^C(\mathbf{r}; \omega) = \epsilon(\mathbf{r}; \omega) + \frac{i}{\epsilon_0\omega}\sigma(\mathbf{r}; \omega) \quad (19.16)$$

is the so-called complex (C) relative dielectric constant.

19.1.2 Eikonal Equation and Energy Transport

To derive the short-wavelength approximation to the macroscopic Maxwell equations let us write the $\mathbf{E}$ - and $\mathbf{H}$ -fields in the form

$$\mathbf{E}(\mathbf{r}; \omega) = \mathbf{E}^0(\mathbf{r}; \omega) \exp(iq_0 S(\mathbf{r}; \omega)), \quad (19.17)$$

$$\mathbf{H}(\mathbf{r}; \omega) = \mathbf{H}^0(\mathbf{r}; \omega) \exp(iq_0 S(\mathbf{r}; \omega)). \quad (19.18)$$

The vectorial “amplitudes” $\mathbf{E}^0(\mathbf{r}; \omega)$ and $\mathbf{H}^0(\mathbf{r}; \omega)$, and the scalar “phase” $S(\mathbf{r}; \omega)$, are not uniquely defined by the ansatz’s above, and $S(\mathbf{r}; \omega)$ in general has both real and imaginary parts. As indicated in the notation, the various quantities depend on both position and frequency. By inserting (19.17) and (19.18) into the Maxwell equations in (19.12)–(19.15) these take the form

$$iq_0 (\nabla S \times \mathbf{E}^0 - c_0 \mu_0 \mu \mathbf{H}^0) = -\nabla \times \mathbf{E}^0, \quad (19.19)$$

$$iq_0 (\nabla S \times \mathbf{H}^0 + c_0 \epsilon_0 \epsilon^C \mathbf{E}^0) = -\nabla \times \mathbf{H}^0, \quad (19.20)$$

$$iq_0 \epsilon^C \nabla S \cdot \mathbf{E}^0 = -\epsilon^C \nabla \cdot \mathbf{E}^0 - \nabla \epsilon^C \cdot \mathbf{E}^0, \quad (19.21)$$

$$iq_0 \mu \nabla S \cdot \mathbf{H}^0 = -\mu \nabla \cdot \mathbf{H}^0 - \nabla \mu \cdot \mathbf{H}^0. \quad (19.22)$$

Since the quantities on the right-hand side of these equations for physical reasons always are finite, the macroscopic Maxwell equations in (19.19)–(19.22) reduce for sufficiently high frequencies ($q_0 \rightarrow \infty$) to

$$\nabla S(\mathbf{r}; \omega) \times \mathbf{E}^0(\mathbf{r}; \omega) = c_0 \mu_0 \mu(\mathbf{r}; \omega) \mathbf{H}^0(\mathbf{r}; \omega), \quad (19.23)$$

$$\nabla S(\mathbf{r}; \omega) \times \mathbf{H}^0(\mathbf{r}; \omega) = -c_0 \epsilon_0 \epsilon^C(\mathbf{r}; \omega) \mathbf{E}^0(\mathbf{r}; \omega), \quad (19.24)$$

$$\nabla S(\mathbf{r}; \omega) \cdot \mathbf{E}^0(\mathbf{r}; \omega) = 0, \quad (19.25)$$

$$\nabla S(\mathbf{r}; \omega) \cdot \mathbf{H}^0(\mathbf{r}; \omega) = 0. \quad (19.26)$$

The reader may notice that (19.25) and (19.26) follow from (19.23) and (19.24) on scalar multiplication with $\nabla S(\mathbf{r}; \omega)$ (just as (19.14) and (19.15) follow from (19.12) and (19.13) by taking the divergence). One can therefore confine the attention to (19.23) and (19.24). The function $S(\mathbf{r}; \omega)$ is usually called the eikonal, and it appears from (19.25) and (19.26) that the field amplitudes $\mathbf{E}^0(\mathbf{r}; \omega)$ and $\mathbf{H}^0(\mathbf{r}; \omega)$ everywhere in space are orthogonal to the gradient of the eikonal. Note also that only the gradient of $S(\mathbf{r}; \omega)$ plays a physical role. We shall have more to say on this point soon. Now, one multiplies the two sides of (19.23) vectorially by $\nabla S(\mathbf{r}; \omega)$ from the left. This gives upon use of (19.24)

$$\nabla S \times (\nabla S \times \mathbf{E}^0) = -\epsilon^C \mu \mathbf{E}^0. \quad (19.27)$$

By use of a standard relation for the double vector product and (19.25), one obtains upon elimination of $\mathbf{E}^0$ from (19.27) what may be called the complex eikonal equation

$$\nabla S(\mathbf{r}; \omega) \cdot \nabla S(\mathbf{r}; \omega) = n^2(\mathbf{r}; \omega), \quad (19.28)$$

where

$$n(\mathbf{r}; \omega) = \left(\epsilon^C(\mathbf{r}; \omega) \mu(\mathbf{r}; \omega) \right)^{1/2} \quad (19.29)$$

is the complex refractive index of macroscopic electrodynamics. By division of $S(\mathbf{r}; \omega)$ and $n(\mathbf{r}; \omega)$ into their real (R) and imaginary (I) parts, i.e., $S = S_R + iS_I$ and $n = n_R + i n_I$, (19.28) divides as follows:

$$\nabla S_R(\mathbf{r}; \omega) \cdot \nabla S_R(\mathbf{r}; \omega) - \nabla S_I(\mathbf{r}; \omega) \cdot \nabla S_I(\mathbf{r}; \omega) = n_R^2(\mathbf{r}; \omega) - n_I^2(\mathbf{r}; \omega), \quad (19.30)$$

$$\nabla S_R(\mathbf{r}; \omega) \cdot \nabla S_I(\mathbf{r}; \omega) = n_R(\mathbf{r}; \omega)n_I(\mathbf{r}; \omega). \quad (19.31)$$

Geometrical optics most often is used to study optical properties in nonconducting media ($\sigma(\mathbf{r}; \omega) = 0$), and in cases where also the imaginary parts of the dielectric permittivity and the magnetic permeability are negligible. When the above-mentioned criteria are satisfied, the refractive index and the eikonal become real quantities, i.e., $n(\mathbf{r}; \omega) \approx n_R(\mathbf{r}; \omega)$ and $S(\mathbf{r}; \omega) \approx S_R(\mathbf{r}; \omega)$, and the quantity $\exp(iq_0 S(\mathbf{r}; \omega))$ in (19.17) and (19.18) then is a genuine phase factor. For real $n(\mathbf{r}; \omega)$, the surfaces $S(\mathbf{r}; \omega) = \text{constant}$ are called the geometrical wave surfaces (or wave fronts).

In the remaining part of this subsection, it is assumed that the relative permittivity and permeability are real quantities. We denote these by $\tilde{\epsilon}$ and $\tilde{\mu}$, and remark that even the so-called complex dielectric constant ϵ^C (19.16) may be real provided the conductivity is purely imaginary (and ϵ is real). For sufficiently high frequencies, where the diamagnetic response dominates, σ is in fact a purely imaginary quantity. It follows from elementary analyses that the cycle-averaged ($\langle \dots \rangle$) energy density in the electromagnetic field

$$\langle W(\mathbf{r}, t) \rangle = \langle W_e(\mathbf{r}, t) \rangle + \langle W_m(\mathbf{r}, t) \rangle, \quad (19.32)$$

as indicated, is the sum of electric (e) and magnetic (m) parts, which are given by

$$\langle W_e(\mathbf{r}, t) \rangle = \frac{1}{4} \epsilon_0 \tilde{\epsilon}(\mathbf{r}; \omega) \mathbf{E}(\mathbf{r}; \omega) \cdot \mathbf{E}^*(\mathbf{r}; \omega), \quad (19.33)$$

and

$$\langle W_m(\mathbf{r}, t) \rangle = \frac{1}{4} \mu_0 \tilde{\mu}(\mathbf{r}; \omega) \mathbf{H}(\mathbf{r}; \omega) \cdot \mathbf{H}^*(\mathbf{r}; \omega), \quad (19.34)$$

and are equal in magnitude, i.e.,

$$\langle W_e(\mathbf{r}, t) \rangle = \langle W_m(\mathbf{r}, t) \rangle. \quad (19.35)$$

In the macroscopic theory, the cycle-averaged Poynting vector is

$$\langle \mathbf{S}(\mathbf{r}, t) \rangle = \frac{1}{4} (\mathbf{E}(\mathbf{r}; \omega) \times \mathbf{H}^*(\mathbf{r}; \omega) + c.c.). \quad (19.36)$$

A real refractive index, $\tilde{n} = (\tilde{\epsilon}\tilde{\mu})^{1/2}$, implies that the eikonal $S(\mathbf{r}; \omega)$ also is real, and (19.17) and (19.18) then show that

$$\langle \mathbf{S}(\mathbf{r}, t) \rangle = \frac{1}{4} \left\{ \mathbf{E}^0(\mathbf{r}; \omega) \times [\mathbf{H}^0(\mathbf{r}; \omega)]^* + c.c. \right\}. \quad (19.37)$$

The Poynting vector can be related to the gradient of the eikonal by inserting the expression for $\mathbf{H}^0$ given in (19.23) into (19.37). With $\mu \approx \tilde{\mu}$, one thus obtains

$$\langle S(\mathbf{r}, t) \rangle = \frac{1}{4c_0\mu_0\tilde{\mu}} [E^0 \cdot (E^0)^* \nabla S - (E^0)^* E^0 \cdot \nabla S + c.c.] \quad (19.38)$$

in the geometrical optical limit. The middle term in the parenthesis vanishes because of (19.25), and the first term is real. Therefore, one finds

$$\langle S(\mathbf{r}, t) \rangle = \frac{1}{2c_0\mu_0\tilde{\mu}} E^0 \cdot (E^0)^* \nabla S. \quad (19.39)$$

The cycle-averaged energy density in the electromagnetic field can at high frequencies be written in the form

$$\langle W(\mathbf{r}, t) \rangle = \frac{1}{2} \epsilon_0 \tilde{\epsilon} E^0 \cdot (E^0)^*, \quad (19.40)$$

as the reader may realize by combining (19.32)–(19.34), and utilizing the eikonal form given in (19.17) and (19.18). From (19.39) and (19.40), one next obtains

$$\langle S(\mathbf{r}, t) \rangle = c_0 \tilde{n}^{-2} \langle W(\mathbf{r}, t) \rangle \nabla S(\mathbf{r}; \omega). \quad (19.41)$$

The eikonal equation, when written in the form

$$\frac{\nabla S}{\tilde{n}} \cdot \frac{\nabla S}{\tilde{n}} = 1, \quad (19.42)$$

tells us that

$$\hat{\mathbf{u}} = \tilde{n}^{-1} \nabla S \quad (19.43)$$

is a local unit vector perpendicular to the geometrical wave front at $\mathbf{r}$. In terms of this unit vector, (19.41) finally becomes

$$\langle S(\mathbf{r}, t) \rangle = \frac{c_0}{\tilde{n}} \langle W(\mathbf{r}, t) \rangle \hat{\mathbf{u}}(\mathbf{r}; \omega). \quad (19.44)$$

Hence, the cycle-averaged Poynting vector is everywhere in space in the direction of the normal to the geometrical wave surface, and the cycle-averaged energy density is propagated with the velocity $c_0/\tilde{n}$ in the framework of geometrical optics.

19.2 Massive Transverse Photon

19.2.1 Microscopic Transverse Electrodynamics at High Frequencies

The particle-wave duality in quantum mechanics implies that transverse photons in observations can appear wave- or particle-like. At high frequencies the particle

behavior tends to dominate. In a sense one may, therefore, claim that geometrical optics deals with the propagation of light particles. During the transport of these particles through a medium the field–matter interaction causes the transverse photons to appear with an effective rest mass. To discuss the mass concept of transverse photons within the framework of photon wave mechanics, we start from the transverse set of Maxwell–Lorentz equations, which in the space–frequency domain take the form

$$\nabla \times \mathbf{E}_T(\mathbf{r}; \omega) = i\omega \mathbf{B}(\mathbf{r}; \omega), \quad (19.45)$$

$$\nabla \times \mathbf{B}(\mathbf{r}; \omega) = \mu_0 \mathbf{J}_T(\mathbf{r}; \omega) - i\omega c_0^{-2} \mathbf{E}_T(\mathbf{r}; \omega), \quad (19.46)$$

cf. (9.25) and (9.26). Beforehand, one would expect that a photon mass concept makes sense only in relation to linear response theory, and we shall realize shortly that this assertion is correct. Limiting ourselves to condensed matter media with dominating (many-body) electron response, it was shown in Sect. 12.5 that the diamagnetic coupling dominates the field–matter interaction at high frequencies. Using the local form of the diamagnetic response tensor (last term of (12.79)) the constitutive equation becomes

$$\mathbf{J}(\mathbf{r}; \omega) = \frac{ie^2}{m\omega} N_0(\mathbf{r}) \mathbf{E}_T(\mathbf{r}; \omega), \quad \omega \rightarrow \infty. \quad (19.47)$$

It is useful here to relate the diamagnetic current density to the transverse part of the vector potential instead of to $\mathbf{E}_T(\mathbf{r}; \omega)$. Hence,

$$\mathbf{J}(\mathbf{r}; \omega) = -\frac{e^2}{m} N_0(\mathbf{r}) \mathbf{A}_T(\mathbf{r}; \omega), \quad \omega \rightarrow \infty. \quad (19.48)$$

It appears from this equation that the factor which relates $\mathbf{A}_T(\mathbf{r}; \omega)$ to $\mathbf{J}(\mathbf{r}; \omega)$ is independent of the frequency of the electromagnetic field. It is this fact which gives transverse photons an effective mass at high frequencies, as we shall see soon. The transverse part of the vector potential satisfies the inhomogeneous wave equation

$$(\nabla^2 + q_0^2) \mathbf{A}_T(\mathbf{r}; \omega) = -\mu_0 \mathbf{J}_T(\mathbf{r}; \omega) \quad (19.49)$$

in the space–frequency domain, cf. (9.44), and if the transverse delta function is used to project out $\mathbf{J}_T(\mathbf{r}; \omega)$ from (19.48), one obtains the following integro-differential equation for $\mathbf{A}_T(\mathbf{r}; \omega)$:

$$(\nabla^2 + q_0^2) \mathbf{A}_T(\mathbf{r}; \omega) = \frac{\mu_0 e^2}{m} \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot [N_0(\mathbf{r}') \mathbf{A}_T(\mathbf{r}'; \omega)] d^3 r'. \quad (19.50)$$

Equation (19.50) is a good starting point for theoretical studies of the high-frequency field–matter interaction in semiclassical electrodynamics.

19.2.2 *Quantum Mechanical Photon Wave Equation in a Homogeneous Medium*

In photon wave mechanics, analytical signals play the key role, and it is therefore natural already at this stage to assume that the angular frequency in (19.50) is positive. The homogeneity of the integro-differential equation in (19.50) implies that the magnitude of the transverse vector potential is arbitrary. In the following we shall assume that we are dealing with one-photon amplitudes, and thus make the usual replacement $\mathbf{A}_T^{(+)}(\mathbf{r}; \omega) \Rightarrow \mathbf{a}_T^{(+)}(\mathbf{r}; \omega)$. In the context of wave mechanics of transverse photons, (19.50) hence is replaced by

$$(\nabla^2 + q_0^2) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) = \frac{\mu_0 e^2}{m} \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \left[N_0(\mathbf{r}') \mathbf{a}_T^{(+)}(\mathbf{r}'; \omega) \right] d^3 r'. \quad (19.51)$$

Before proceeding it is worth emphasizing that the “propagation” of transverse photons through a condensed matter medium involves a repeated absorption and reemission of “genuine” photons, and the words “one-photon amplitude” thus must be taken with a grain of salt.

Let us assume now that the spatial variations in the electron density are negligible. If the uniform electron density is denoted by N_0 , one has

$$\int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \left[N_0(\mathbf{r}; \omega) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) \right] d^3 r' = N_0 \mathbf{a}_T^{(+)}(\mathbf{r}; \omega). \quad (19.52)$$

The approximation in (19.52) reduces (19.51) to the much simpler form

$$(\nabla^2 + q_0^2 - Q_C^2) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) = \mathbf{0}, \quad (19.53)$$

where

$$Q_C = \frac{1}{c_0} \left(\frac{N_0 e^2}{m \epsilon_0} \right)^{1/2} \quad (19.54)$$

is the plasma wave number of the homogeneous electron system. For a reason that will become obvious soon the plasma wave number has been given a subscript C. Transferred to the space–time domain (19.53) becomes

$$\left(\nabla^2 - Q_C^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{a}_T^{(+)}(\mathbf{r}, t) = \mathbf{0}, \quad (19.55)$$

and if one, in analogy to what was done in Sect. 16.4.1, formally factorizes the operator acting on $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$ one may write (19.55) as follows:

$$\left(\sqrt{Q_C^2 - \nabla^2} + \frac{i}{c_0} \frac{\partial}{\partial t} \right) \left(\sqrt{Q_C^2 - \nabla^2} - \frac{i}{c_0} \frac{\partial}{\partial t} \right) \mathbf{a}_T^{(+)}(\mathbf{r}, t) = \mathbf{0}. \quad (19.56)$$

The nonlocal operator $(Q_C^2 - \nabla^2)^{1/2}$ is defined via its action in reciprocal space, i.e.,

$$\sqrt{Q_C^2 - \nabla^2} F(\mathbf{r}) = \int_{-\infty}^{\infty} \sqrt{Q_C^2 + q^2} F(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} \frac{d^3 q}{(2\pi)^3}, \quad (19.57)$$

cf. (15.21). Every solution to

$$i\hbar \frac{\partial}{\partial t} \mathbf{a}_T^{(+)}(\mathbf{r}, t) = c_0 \hbar \sqrt{Q_C^2 - \nabla^2} \mathbf{a}_T^{(+)}(\mathbf{r}, t) \quad (19.58)$$

is also a solution to (19.56), and (19.58) may be considered as the quantum mechanical wave equation for a transverse photon propagating through a uniform medium. Equivalently, $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$ can be characterized as the wave function of a polariton (or plasmariton), the collective field–matter quantum excitation.

19.2.3 Energy–Momentum Relation: Mass of Transverse Photon

With the help of the definition in (19.57) it is easy to see that the quantum mechanical wave equation for the transverse photon in the wave vector–time domain takes the form

$$i\hbar \frac{\partial}{\partial t} \mathbf{a}_T^{(+)}(\mathbf{q}; t) = H(\mathbf{q}) \mathbf{a}_T^{(+)}(\mathbf{q}; t), \quad (19.59)$$

where

$$H(\mathbf{q}) = c_0 \hbar \sqrt{q^2 + Q_C^2} \quad (19.60)$$

is the particle’s Hamilton operator. The monochromatic $(\exp(-i\omega t))$ stationary-state solutions to (19.59) satisfy the dispersion relation

$$\omega = c_0 \sqrt{q^2 + Q_C^2}, \quad (19.61)$$

which, by means of the Einstein–de Broglie relations in (15.2) and (15.3), is equivalent to the particle energy–momentum relation

$$E = +\sqrt{(pc_0)^2 + (\hbar c_0 Q_C)^2}. \quad (19.62)$$

Upon a comparison of this equation to the relation in (15.4) one may in a sense claim that the transverse photon has acquired a finite (effective) rest mass

$$M = \frac{\hbar Q_C}{c_0} \quad (19.63)$$

due to its high-frequency diamagnetic interaction with the uniform electron system. The quantity

$$Q_C = \frac{Mc_0}{\hbar} \quad (19.64)$$

hence is the Compton (C) wave number of the massive photon. Expressed in terms of the many-body electron density, $\mathcal{N}_0$, the mass of the transverse photon is

$$M = \frac{\hbar}{c_0^2} \left(\frac{\mathcal{N}_0 e^2}{m \epsilon_0} \right)^{1/2}. \quad (19.65)$$

The mass, thus, increases proportional to the square root of the electron density.

19.2.4 Photon Mass in the Energy Wave Function Formalism

The studies in the previous two subsections have led to the conclusion that a transverse photon, if characterized in the potential theory by the wave function $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$, acquires a finite mass in its propagation through a homogeneous electron system. Since the transverse vector potential is gauge invariant, the transverse mass concept is not a gauge dependent property, and it is plausible therefore that the same finite mass also will appear in the framework of the photon energy wave function formalism.

In order to elucidate this point let us return to the dynamical equations for the transverse field, i.e., (19.45) and (19.46). Being interested in one-photon dynamics we make the usual replacements $\mathbf{E}_T(\mathbf{r}; \omega) \Rightarrow \mathbf{e}_T^{(+)}(\mathbf{r}; \omega)$, $\mathbf{B}(\mathbf{r}; \omega) \Rightarrow \mathbf{b}^{(+)}(\mathbf{r}; \omega)$ and $\mathbf{J}_T(\mathbf{r}; \omega) \Rightarrow \mathcal{J}_T^{(+)}(\mathbf{r}; \omega)$ in these equations. In the relation

$$\nabla \times \mathbf{b}^{(+)}(\mathbf{r}; \omega) = \mu_0 \mathcal{J}_T^{(+)}(\mathbf{r}; \omega) - i\omega c_0^{-2} \mathbf{e}_T^{(+)}(\mathbf{r}; \omega), \quad (19.66)$$

we now eliminate $\mathbf{e}_T^{(+)}(\mathbf{r}; \omega)$ and $\mathcal{J}_T^{(+)}(\mathbf{r}; \omega)$ in favor of the analytical vector potential $\mathbf{a}_T^{(+)}(\mathbf{r}; \omega)$. For a homogeneous electron system, where $N_0(\mathbf{r}) = \mathcal{N}_0$, it is clear that the high-frequency current density given by the expression in (19.48) is a transverse vector field. In turn, this implies that

$$\mathcal{J}_T^{(+)}(\mathbf{r}; \omega) = -\frac{e^2}{m} \mathcal{N}_0 \mathbf{a}_T^{(+)}(\mathbf{r}; \omega), \quad (19.67)$$

and if this equation together with the relation $\mathbf{e}_T^{(+)}(\mathbf{r}; \omega) = i\omega \mathbf{a}_T^{(+)}(\mathbf{r}; \omega)$ are inserted in (19.66) one obtains

$$\nabla \times \mathbf{b}^{(+)}(\mathbf{r}; \omega) = (q_0^2 - Q_C^2) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega). \quad (19.68)$$

By taking the curl on the two sides of (19.68), the reader may verify that the following wave equation is obtained for the magnetic field:

$$\nabla^2 \mathbf{b}^{(+)}(\mathbf{r}; \omega) = (Q_C^2 - q_0^2) \mathbf{b}^{(+)}(\mathbf{r}; \omega). \quad (19.69)$$

The curl of the one-photon version of (19.45) gives upon use of (19.68) the expected wave equation for $\mathbf{e}_T^{(+)}(\mathbf{r}; \omega)$, namely

$$\nabla^2 \mathbf{e}_T^{(+)}(\mathbf{r}; \omega) = (Q_C^2 - q_0^2) \mathbf{e}_T^{(+)}(\mathbf{r}; \omega). \quad (19.70)$$

The form-identity of the wave equations for $\mathbf{e}_T^{(+)}(\mathbf{r}; \omega)$ and $\mathbf{b}^{(+)}(\mathbf{r}; \omega)$ immediately enables one to set up wave equations for the one-photon Riemann–Silberstein vectors, which in the space–frequency domain are given by

$$f_{\pm}^{(+)}(\mathbf{r}; \omega) = \sqrt{\frac{\epsilon_0}{2}} \left(\mathbf{e}_T^{(+)}(\mathbf{r}; \omega) \pm i c_0 \mathbf{b}^{(+)}(\mathbf{r}; \omega) \right). \quad (19.71)$$

Thus, one obtains

$$(\nabla^2 + q_0^2 - Q_C^2) \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) = \mathbf{0}. \quad (19.72)$$

Since the differential equation for the two photon helicity states has the same form as the one for the one-photon vector potential $\mathbf{a}_T^{(+)}(\mathbf{r}; \omega)$, see (19.53), one necessarily ends up with the following Schrödinger-like quantum mechanical wave equation for the two energy wave function species in space–time:

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = c_0 \hbar \sqrt{Q_C^2 - \nabla^2} \mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t), \quad (19.73)$$

cf. (19.58). In the wave-vector representation, one finally gets the (identical) quantum mechanical wave equations

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) = c_0 \hbar \sqrt{q^2 + Q_C^2} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) \quad (19.74)$$

for the two helicity components. On the basis of (19.74) one therefore may conclude that the transverse photon in its propagation through a homogeneous electron system acquires the same effective mass $M = \hbar Q_C / c_0$ in the potential and energy wave function descriptions, a satisfactory result.

It is possible also to introduce the helicity operator concept in the massive photon theory. To achieve this goal we first use (15.72) to rewrite (19.74) in the distinct forms

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) = \pm i c_0 \hbar (q^2 + Q_C^2)^{1/2} \hat{\mathbf{q}} \times \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t). \quad (19.75)$$

With the help of (15.109), the Cartesian spin-one operator, $\hat{\mathbf{s}}$, is brought into play. Thus, one obtains

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) = \pm c_0 \left[1 + \left(\frac{Q_C}{q} \right)^2 \right]^{1/2} \left(\frac{\hat{\mathbf{s}}}{\hbar} \cdot \hbar \mathbf{q} \right) \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t), \quad (19.76)$$

and then in terms of the matrix representative of the photon helicity operator, $\mathbf{h}$, given in (17.72), one finally is led to the dynamical equations

$$i\hbar \frac{\partial}{\partial t} \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t) = \pm c_0 (q^2 + Q_C^2)^{1/2} \mathbf{h} \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t). \quad (19.77)$$

In the limit $Q_C \rightarrow 0$, (19.77) is reduced to the corresponding free-photon Schrödinger equations, written down explicitly in the complex field theory in (17.71). As already emphasized in Sect. 17.3.4, equations form-identical to (17.71) hold for the energy wave functions $\mathbf{f}_{\pm}^{(+)}(\mathbf{q}; t)$.

19.3 Photon Eikonal Gradient: Local Particle Momentum

19.3.1 Photon Eikonal Equation

Let us now return to the fundamental integro-differential equation for the one-photon vector potential $\mathbf{a}_T^{(+)}(\mathbf{r}; \omega)$ (19.51), and here make the eikonal ansatz

$$\mathbf{a}_T^{(+)}(\mathbf{r}; \omega) = \mathbf{a}^0 \exp(iq_0 S(\mathbf{r}; \omega)). \quad (19.78)$$

By keeping only the highest (second-order) terms in q_0 , the left-hand side of (19.51) reduces in the high frequency limit to

$$(\nabla^2 + q_0^2) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) \approx q_0^2 (1 - \nabla S(\mathbf{r}; \omega) \cdot \nabla S(\mathbf{r}; \omega)) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega). \quad (19.79)$$

The approximate character of (19.79) is apparent from the fact that the left side is divergence-free whereas the right side has a nonvanishing divergence $-q_0^2 \nabla(\nabla S \cdot \nabla S) \cdot \mathbf{a}_T^{(+)}$. On the right-hand side of (19.51) it is assumed that the electron density varies so slowly in space that it is essentially constant over the effective (near-field) range of the transverse delta function. Setting $N_0(\mathbf{r}') \approx N_0(\mathbf{r})$, one obtains

$$\int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \left[N_0(\mathbf{r}') \mathbf{a}_T^{(+)}(\mathbf{r}'; \omega) \right] d^3 r' \approx N_0(\mathbf{r}) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega), \quad (19.80)$$

since $\delta_T(\mathbf{r} - \mathbf{r}')$ projects out the transverse part of $\mathbf{a}_T^{(+)}(\mathbf{r}'; \omega)$ at $\mathbf{r}$, which is $\mathbf{a}_T^{(+)}$ itself at this space point. Also in (19.80), the divergence-free left side is approximated by an expression of nonzero divergence. This is of course necessary in

order for the two approximations in (19.79) and (19.80) to fit together. Equalizing these, one gets after a little algebra the following eikonal equation for the transverse photon:

$$\nabla S(\mathbf{r}; \omega) \cdot \nabla S(\mathbf{r}; \omega) = 1 - \left(\frac{\Omega_p(\mathbf{r})}{\omega} \right)^2, \quad (19.81)$$

where

$$\Omega_p(\mathbf{r}) = \left(\frac{N_0(\mathbf{r})e^2}{m\epsilon_0} \right)^{1/2} \quad (19.82)$$

is the local (space-dependent) many-body cyclic plasma frequency.

As the reader perhaps would expect, the same eikonal equation, as derived above on the basis of the potential theory, can also be obtained starting from the energy wave function formalism for the transverse photon variables $\mathbf{f}_{\pm}^{(+)}$. In order to show this we begin with the two inhomogeneous wave equations

$$(\nabla^2 + q_0^2) \mathbf{e}_T^{(+)}(\mathbf{r}; \omega) = -i\mu_0\omega \mathcal{J}_T^{(+)}(\mathbf{r}; \omega), \quad (19.83)$$

$$(\nabla^2 + q_0^2) \mathbf{b}^{(+)}(\mathbf{r}; \omega) = -\mu_0 \nabla \times \mathcal{J}_T^{(+)}(\mathbf{r}; \omega). \quad (19.84)$$

From these we immediately obtain the two equations

$$(\nabla^2 + q_0^2) \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) = -i\mu_0 \sqrt{\frac{\epsilon_0}{2}} \left(\omega \mathcal{J}_T^{(+)}(\mathbf{r}; \omega) \pm c_0 \nabla \times \mathcal{J}_T^{(+)}(\mathbf{r}; \omega) \right) \quad (19.85)$$

for the Riemann–Silberstein vectors. The approximation in (19.80) gives

$$\mathcal{J}_T^{(+)}(\mathbf{r}; \omega) \approx -\frac{e^2}{m} N_0(\mathbf{r}) \mathbf{a}_T^{(+)}(\mathbf{r}; \omega), \quad (19.86)$$

and thereafter

$$\begin{aligned} \nabla \times \mathcal{J}_T^{(+)}(\mathbf{r}; \omega) &\approx -\frac{e^2}{m} \left(\nabla N_0(\mathbf{r}) \times \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) + N_0(\mathbf{r}) \nabla \times \mathbf{a}_T^{(+)}(\mathbf{r}; \omega) \right) \\ &\approx -\frac{e^2}{m} N_0(\mathbf{r}) \mathbf{b}^{(+)}(\mathbf{r}; \omega), \end{aligned} \quad (19.87)$$

since at high frequencies

$$\frac{|\nabla \times \mathbf{a}_T^{(+)}|}{|\mathbf{a}_T^{(+)}|} \sim q_0 |\nabla S| \gg \frac{|\nabla N_0|}{N_0}. \quad (19.88)$$

On the basis of the approximations in (19.86) and (19.87) the terms in the parenthesis on the right side of (19.85) become

$$\omega \mathcal{J}_T^{(+)} \pm c_0 \nabla \times \mathcal{J}_T^{(+)} \approx \frac{ie^2}{m} N_0 \left(i\omega \mathbf{a}_T^{(+)} \pm ic_0 \mathbf{b}^{(+)} \right) = \frac{ie^2}{m} N_0 \left(\frac{2}{\epsilon_0} \right)^{1/2} \mathbf{f}_{\pm}^{(+)}. \quad (19.89)$$

By means of the two eikonal forms

$$\mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) = \mathbf{F}_{\pm}(\mathbf{r}; \omega) \exp(iq_0 S_{\pm}(\mathbf{r}; \omega)), \quad (19.90)$$

we obtain at high frequencies

$$(\nabla^2 + q_0^2) \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \approx q_0^2 (1 - \nabla S_{\pm}(\mathbf{r}; \omega) \cdot \nabla S_{\pm}(\mathbf{r}; \omega)) \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega). \quad (19.91)$$

A combination of (19.85), (19.89) and (19.91) finally leads to the conclusion that the two helicity states have the same eikonal, i.e.,

$$S_+(\mathbf{r}; \omega) = S_-(\mathbf{r}; \omega) \equiv S(\mathbf{r}; \omega), \quad (19.92)$$

and that the eikonal $S(\mathbf{r}; \omega)$ satisfies the eikonal equation in (19.81). Since the diamagnetic electron response only depends on the electron density $N_0(\mathbf{r})$, it is perhaps not surprising that the two photon helicity species have the same eikonal equation.

19.3.2 Local Photon Momentum

In the view of (16.53), it follows from (16.51) that the transverse photon momenta of the two helicity species in the monochromatic case, where

$$\mathbf{f}_{\pm}^{(+)}(\mathbf{r}, t) = \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) e^{-i\omega t}, \quad (19.93)$$

are given by

$$\mathbf{P}_{\pm} = \pm \frac{1}{ic_0} \int_{-\infty}^{\infty} \left[\mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \right]^* \times \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) d^3r, \quad (19.94)$$

or equivalently by

$$\mathbf{P}_{\pm} = \pm \frac{1}{ic_0} \int_{-\infty}^{\infty} \mathbf{F}_{\pm}^*(\mathbf{r}; \omega) \times \mathbf{F}_{\pm}(\mathbf{r}; \omega) d^3r \quad (19.95)$$

since the (identical) eikonals in (19.90) are real quantities. The eikonal gradient can be introduced in (19.95) with the help of the dynamical equations for the energy wave function variables. Since the one-photon current density in (18.27) only gives a small correction to the free wave equations

$$q_0 \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) = \pm \nabla \times \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \quad (19.96)$$

in the eikonal limit, it is sufficient here to insert the ansatz's in (19.90) into (19.96). For $q_0 \rightarrow \infty$, one thus obtains the relations

$$\mathbf{F}_{\pm}(\mathbf{r}; \omega) = \pm i \nabla S(\mathbf{r}; \omega) \times \mathbf{F}_{\pm}(\mathbf{r}; \omega). \quad (19.97)$$

By inserting the above expressions for the $\mathbf{F}_{\pm}$'s into the last factor under the integral sign in (19.95), and utilizing that

$$\mathbf{F}_{\pm}(\mathbf{r}; \omega) \cdot \nabla S(\mathbf{r}; \omega) = 0, \quad (19.98)$$

a result which readily follows from (19.97), one obtains

$$\mathbf{P}_{\pm} = c_0^{-1} \int_{-\infty}^{\infty} \mathbf{F}_{\pm}^*(\mathbf{r}; \omega) \cdot \mathbf{F}_{\pm}(\mathbf{r}; \omega) \nabla S(\mathbf{r}; \omega) d^3 r, \quad (19.99)$$

and then

$$\mathbf{P}_{\pm} = c_0^{-1} \int_{-\infty}^{\infty} \left[\mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \right]^* \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \nabla S(\mathbf{r}; \omega) d^3 r. \quad (19.100)$$

With the help of (19.43), the photon momenta finally may be written in the form

$$\mathbf{P}_{\pm} = \int_{-\infty}^{\infty} \frac{\left[\mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega) \right]^* \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega)}{c_0 / \tilde{n}(\mathbf{r}; \omega)} \hat{\mathbf{u}}(\mathbf{r}; \omega) d^3 r, \quad (19.101)$$

where

$$\tilde{n}(\mathbf{r}; \omega) = \left[1 - \left(\frac{\Omega_p(\mathbf{r})}{\omega} \right)^2 \right]^{1/2} \quad (19.102)$$

is the microscopic refractive index in the eikonal limit. The result in (19.101) has a clear physical interpretation. Since (16.38) shows that $[\mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega)] \cdot \mathbf{f}_{\pm}^{(+)}(\mathbf{r}; \omega)$ are the local energy probabilities of the two helicity species, and $c_0 / \tilde{n}(\mathbf{r}; \omega)$ is the local propagation speed of these probabilities, the quantities in front of the local unit vector $\hat{\mathbf{u}}(\mathbf{r}; \omega)$ are just the magnitude of the local momentum density of the helicity species. The propagation direction of the local momentum densities is given by the unit vector $\hat{\mathbf{u}}(\mathbf{r}; \omega)$. A schematic illustration of the motion of a massive transverse photon along a trajectory is shown in Fig. 19.1.

If the spatial variation in the electron density is negligible, so that $N_0(\mathbf{r}) \approx \mathcal{N}_0$, it is obvious from (19.81) that the eikonal gradient must have the same direction everywhere in space. Let this direction be given by the unit vector $\hat{\mathbf{k}}$. From the equation

$$\nabla S(\mathbf{r}; \omega) = \left[1 - \left(\frac{Q_c}{q_0} \right)^2 \right]^{1/2} \hat{\mathbf{k}} \equiv \tilde{n}_0(\omega) \hat{\mathbf{k}}, \quad (19.103)$$

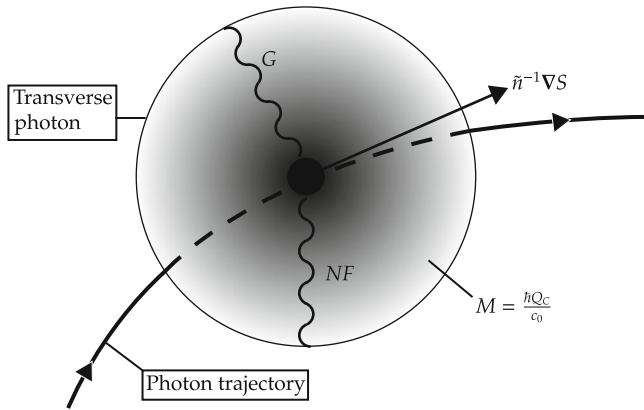


Fig. 19.1 In matter, the spatial localization of a transverse photon is limited by its interaction with near-field (NF) and gauge (G) photons. At *high* frequencies, where the field–matter interaction is diamagnetic, the transverse photon has an effective mass $M = \hbar Q_C/c_0$, and the particle-like object can propagate along a trajectory with local unit vector $\tilde{n}^{-1}\nabla S$. In the de Broglie–Bohm causal interpretation of quantum mechanics a trajectory description is formulated for *massive* particles, even in many body quantum mechanics [259–263]. Whether any means can be found to give substance to the notion of a trajectory description for massless particles is unknown [264, 265]. In the perspective of near-field electrodynamic problems, the possibilities for establishing a trajectory theory for the elusive photon have been discussed recently [254]

the reader may easily convince himself that the general solution for the eikonal is

$$S(\mathbf{r}; \omega) = \tilde{n}_0(\omega) \hat{\mathbf{k}} \cdot \mathbf{r} + S_0(\omega), \quad (19.104)$$

where $S_0(\omega)$ is an arbitrary space-independent constant.

19.4 Hamilton–Jacobi Formulation of Classical Mechanics

In the eikonal limit photon wave mechanics shows a striking connection to the classical mechanics of a point particle. The microscopic eikonal equation for the photon, viz.,

$$\nabla S(\mathbf{r}; \omega) \cdot \nabla S(\mathbf{r}; \omega) = \tilde{n}^2(\mathbf{r}; \omega), \quad (19.105)$$

thus turns out to be form-identical to the Hamilton–Jacobi equation for the characteristic function of a single classical particle. Starting from the Lagrange formulation of Newtonian mechanics we shall in this section briefly recall the steps leading to the Hamilton–Jacobi equations for Hamilton’s principal (S) and characteristic (W) functions.

19.4.1 *The Hamilton Equations and Their Derivation from a Variational Principle*

It is known from elementary classical mechanics that the dynamics of a particle system with n degrees of freedom can be described by n equations of motions of the form ($i = 1, 2, \dots, n$)

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0. \quad (19.106)$$

In these so-called Lagrange equations, the Lagrange function L , which is the difference between the kinetic (T) and potential (V) energies of the system, i.e., $L = T - V$, appears. The Lagrange function

$$L = L(q, \dot{q}, t) \quad (19.107)$$

is a function of the n generalized coordinates

$$q \equiv \{q_i\} = (q_1, q_2, \dots, q_n), \quad (19.108)$$

the associated generalized velocities [$\dot{q}_i \equiv dq_i(t)/dt$]

$$\dot{q} \equiv \{\dot{q}_i\} = (\dot{q}_1, \dot{q}_2, \dots, \dot{q}_n), \quad (19.109)$$

and of time, t . As the Lagrange equations are of second order in time, $2n$ initial values are needed to specify the motion of the system. These may, e.g., be the n q_i 's and the n $\dot{q}_i$'s at a particular time.

In the Hamiltonian formulation, the dynamics of the n -particle system is described via $2n$ first-order equations of motion. To establish these so-called Hamilton equations let us first introduce the generalized (or conjugate) momenta $\{p_i\}$ by the definition

$$p_i = \frac{\partial}{\partial \dot{q}_i} L(q, \dot{q}, t). \quad (19.110)$$

The conjugate momentum p_i is also called the canonical momentum. The canonical momentum concept was introduced already in Sect. 11.4 (11.80), yet in a somewhat different context, and we know from there that it is the conjugate position (q_i) and momentum (p_i) variables which in the quantum theory become operators satisfying the fundamental commutator relations in (11.96) and (11.97). In principle, the n equations in (19.110) allow one to express the generalized velocities in terms of the generalized coordinates and momenta. The Hamilton function (or Hamiltonian), $H(q, p, t)$, is obtained from the Lagrange function (or Lagrangian) by a Legendre transformation

$$H(q, p, t) = \sum_i \dot{q}_i p_i - L(q, \dot{q}, t). \quad (19.111)$$

As indicated, the Hamiltonian in (19.111) is considered to be a function of the conjugate coordinates q (19.108) and momenta

$$p \equiv \{p_i\} = (p_q, p_2, \dots p_n), \quad (19.112)$$

and to achieve this (19.110) is used to eliminate the $\dot{q}_i$'s in favour of the p_i 's. By making use of the definition in (19.110), and the Lagrange equations written with the help of the same equation in the form

$$\frac{\partial}{\partial q_i} L(q, \dot{q}, t) = \dot{p}_i \quad (19.113)$$

one is lead to the well known Hamilton equations of motion, viz.,

$$\dot{q}_i = \frac{\partial}{\partial p_i} H(q, p, t), \quad (19.114)$$

$$\dot{p}_i = -\frac{\partial}{\partial q_i} H(q, p, t). \quad (19.115)$$

The first of these equations give the $\dot{q}_i$'s as functions of (q, p, t) , and form therefore just the inverse of the equations in (19.110).

It is known from elementary analytical mechanics that the Lagrange equations can be derived from Hamilton's variational principle, namely,

$$\delta I \equiv \delta \int_{t_1}^{t_2} L(q, \dot{q}, t) dt = 0. \quad (19.116)$$

The quantity I is referred to as the action or action integral, and Hamilton's principle states that the motion of the system from time t_1 to time t_2 is such that the action I has a stationary value for the correct path of the motion in configuration space (n -dimensional Cartesian hyperspace) where the q 's form the n coordinate axes. Formally, the so-called modified Hamilton principle appears when (19.111) is used to eliminate $L(q, \dot{q}, t)$ in favour of $H(q, p, t)$ in (19.116). Thus,

$$\delta I = \delta \int_{t_1}^{t_2} \left(\sum_i \dot{q}_i p_i - H(q, p, t) \right) dt = 0. \quad (19.117)$$

In (19.117), q and p are treated as independent coordinates of phase space $[(q, p)$ -space], and thus varied independently. The variational principle in (19.117) thus has the form of a variational problem in the $2n$ dimensional phase space, i.e.,

$$\delta I = \delta \int_{t_1}^{t_2} f(q, \dot{q}, p, \dot{p}, t) dt = 0. \quad (19.118)$$

In the usual manner, (19.118) leads to the Lagrange equations ($i = 1, 2, \dots, n$)

$$\frac{d}{dt} \left(\frac{\partial f}{\partial \dot{q}_i} \right) - \frac{\partial f}{\partial q_i} = 0, \quad (19.119)$$

$$\frac{d}{dt} \left(\frac{\partial f}{\partial \dot{p}_i} \right) - \frac{\partial f}{\partial p_i} = 0. \quad (19.120)$$

Since the integrand in (19.117) contains $\dot{q}_i$ only through the $\dot{q}_i p_i$ term, and q_i only in $H(q, p, t)$, (19.119) leads directly to the Hamilton equation in (19.115), and because the integrand in (19.117) does not depend explicitly on $\dot{p}_i$, (19.120) reduces readily to the Hamilton equation in (19.114).

19.4.2 A Particular Canonical Transformation

Let us now consider a simultaneous transformation of the independent phase space coordinates and momenta, q_i, p_i , to a new set Q_i, P_i . The assumed invertible transformation

$$Q_i = Q_i(q, p, t), \quad (19.121)$$

$$P_i = P_i(q, p, t), \quad (19.122)$$

thus defines a transformation of phase space. In the context of Hamiltonian mechanics only those transformations for which the new Q, P -coordinates form a set of conjugate (canonical) variables, are of interest. This is the case provided there exists some new Hamiltonian $K = K(Q, P, t)$ for which the related equations of motion have the Hamiltonian form

$$\dot{Q}_i = \frac{\partial}{\partial P_i} K(Q, P, t), \quad (19.123)$$

$$\dot{P}_i = -\frac{\partial}{\partial Q_i} K(Q, P, t). \quad (19.124)$$

According to the discussion in the previous subsection the Hamilton equations in (19.123) and (19.124) can be derived from the modified Hamilton principle

$$\delta \int_{t_1}^{t_2} \left(\sum_i \dot{Q}_i P_i - K(Q, P, t) \right) dt = 0. \quad (19.125)$$

The statements in (19.117) and (19.125) will both be satisfied if the integrands are connected by a relation of the form

$$\lambda \left(\sum_i \dot{q}_i p_i - H(q, p, t) \right) = \sum_i \dot{Q}_i P_i - K(Q, P, t) + \frac{dF}{dt}, \quad (19.126)$$

where λ is a constant, and F is an arbitrary differentiable function of the phase space coordinates. For what follows it is sufficient to consider canonical transformations for which the scale factor $\lambda = 1$. The function F is a function of (q, p, t) or (Q, P, t) , or any mixture of the phase space coordinates, say (q, Q, t) or (Q, p, t) . The function F is called the generating function of the transformation, and it may act as a bridge between the two sets of canonical variables.

Let us now choose a generating function of the form

$$F = S(q, P, t) - \sum_i Q_i P_i, \quad (19.127)$$

where S , as indicated, is a function of the old coordinates (q) and the new momenta (P). The function S which is called Hamilton's principal function, plays an important role in the formal analogy between the eikonal theory in geometrical optics and classical mechanics as we shall realize soon. Since

$$\frac{dF}{dt} = \frac{dS}{dt} - \sum_i (\dot{Q}_i P_i + Q_i \dot{P}_i), \quad (19.128)$$

and

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \sum_i \left(\frac{\partial S}{\partial q_i} \dot{q}_i + \frac{\partial S}{\partial P_i} \dot{P}_i \right), \quad (19.129)$$

Equation (19.126) takes the particular form

$$\sum_i \left(p_i - \frac{\partial S}{\partial q_i} \right) \dot{q}_i + \sum_i \left(Q_i - \frac{\partial S}{\partial P_i} \right) \dot{P}_i = H - K + \frac{\partial S}{\partial t}. \quad (19.130)$$

Because the right-hand side of (19.130) is independent of the time derivatives $\dot{q}$ and $\dot{P}$, and the old and new coordinates are separately independent, the coefficients of the $\dot{q}_i$'s and $\dot{P}_i$'s in (19.130) both vanish. Hence, one obtains the following equations ($i = 1, 2, \dots, n$)

$$p_i = \frac{\partial}{\partial q_i} S(q, P, t), \quad (19.131)$$

$$Q_i = \frac{\partial}{\partial P_i} S(q, P, t), \quad (19.132)$$

and

$$K(Q, P, t) = H(q, p, t) + \frac{\partial}{\partial t} S(q, P, t). \quad (19.133)$$

19.4.3 Hamilton–Jacobi Equation for Hamilton's Principal Function

If the $2n$ Q_i 's and P_i 's are chosen to be the $2n$ initial values of the q_i 's and p_i 's, and thus time independent, the left sides of (19.123) and (19.124) are both zero. One

can ensure that the new variables are constant in time by requiring that $K(Q, P, t)$ is identically zero. If $q_0 = Q$ and $p_0 = P$ are the initial values of the old phase space variables, then the inverse transformation to the one in (19.121) and (19.122), viz.,

$$q_i = q_i(q_0, p_0, t), \quad (19.134)$$

$$p_i = p_i(q_0, p_0, t), \quad (19.135)$$

is exactly the solution to the mechanical problem under consideration. For $K = 0$, Hamilton's principal function must satisfy the partial differential equation

$$H(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}, t) + \frac{\partial S}{\partial t} = 0. \quad (19.136)$$

Equation (19.136) is the celebrated Hamilton–Jacobi equation for Hamilton's principal function $S(q, P, t)$. Since

$$\frac{dS}{dt} = \sum_i \left(\frac{\partial S}{\partial q_i} \dot{q}_i + \frac{\partial S}{\partial P_i} \dot{P}_i \right) + \frac{\partial S}{\partial t}, \quad (19.137)$$

and $\dot{P}_i = 0$, one obtains with the help of (19.131), (19.136), and the definition of the Hamilton function (19.111)

$$\frac{dS}{dt} = \sum_i p_i \dot{q}_i - H = L. \quad (19.138)$$

The result in (19.138) shows that the principal function of Hamilton differs from the indefinite action integral $I(t)$ at most by a constant (S_0), i.e.,

$$S(q, P, t) = \int L(q, \dot{q}, t) dt + S_0. \quad (19.139)$$

19.4.4 Hamilton–Jacobi Equation for Hamilton's Characteristic Function

In the special, but extremely important, case where the old Hamiltonian H does not depend explicitly on time, the Hamilton–Jacobi equation for Hamilton's principal function becomes

$$H(q_1, \dots, q_n, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_n}) + \frac{\partial S}{\partial t} = 0. \quad (19.140)$$

A trial solution of the form

$$S(q, P, t) = W(q, P) - Et, \quad (19.141)$$

where E is a constant, now is substituted into (19.140). This gives for $W(q, P)$, the so-called characteristic function of Hamilton, a partial differential equation

$$H(q_1, \dots, q_n, \frac{\partial W}{\partial q_1}, \dots, \frac{\partial W}{\partial q_n}) = E, \quad (19.142)$$

which no longer involves any explicit time dependence. For the time independent Hamiltonian in (19.142), the constant E normally will represent the conserved energy of the system, therefore the name E .

19.5 Eikonal Theory of Charged Particles in Quantum Mechanics

19.5.1 Nonrelativistic Hamilton–Jacobi Equation

Let us now consider the single-particle Schrödinger equation for a charged massive particle, viz.,

$$\hat{H}\psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t), \quad (19.143)$$

and let us assume that the particle is placed in an electromagnetic field described by the vector and scalar potentials $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$. In this case the particle's Hamilton operator is given by

$$\hat{H} = \frac{1}{2m} \left(\frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{r}, t) \right)^2 + q\phi(\mathbf{r}, t). \quad (19.144)$$

To understand the way in which the classical equation of motion for the particle emerges from the quantum theory we make the following ansatz for the wave function:

$$\psi(\mathbf{r}, t) = \psi_0 \exp \left(\frac{i}{\hbar} S(\mathbf{r}, t) \right), \quad (19.145)$$

where ψ_0 is a space–time independent constant. By inserting the form in (19.145) into the Schrödinger equation in (19.143) it is not difficult to show that the eikonal $S(\mathbf{r}, t)$ satisfies the partial differential equation

$$\frac{1}{2m} (\nabla S - q\mathbf{A}) \cdot (\nabla S - q\mathbf{A}) + q\phi + \frac{\partial S}{\partial t} = \frac{i\hbar}{2m} \nabla \cdot (\nabla S - q\mathbf{A}). \quad (19.146)$$

Often, (19.146) is called the quantum mechanical Hamilton–Jacobi equation. In general $S(\mathbf{r}, t)$ will be a function of $\hbar$, and if $S(\mathbf{r}, t)$ is expanded in powers of $\hbar/i$, i.e.,

$$S = \sum_{n=0}^{\infty} \left(\frac{\hbar}{i} \right)^n S_n = S_0 + \frac{\hbar}{i} S_1 + \cdots, \quad (19.147)$$

Equation (19.146) becomes a system of coupled equations, one for each power of $\hbar/i$. In the classical limit ($\hbar \rightarrow 0$) only the zeroth order equation,

$$\frac{1}{2m} (\nabla S_0 - q\mathbf{A}) \cdot (\nabla S_0 - q\mathbf{A}) + q\phi + \frac{\partial S_0}{\partial t} = 0, \quad (19.148)$$

survives. This equation is exactly the Hamilton–Jacobi equation for a charged classical particle placed in an electromagnetic field. This is so because with the identification of

$$\mathbf{p} = \nabla S_0 \quad (19.149)$$

as the particle's canonical momentum one obtains the Hamilton function

$$H(\mathbf{r}, \mathbf{p}, t) = \frac{1}{2m} (\mathbf{p} - q\mathbf{A})^2 + q\phi. \quad (19.150)$$

Let us finally show that the Hamilton equations of motions with the $H(\mathbf{r}, \mathbf{p}, t)$ given in (19.150) lead us back to the microscopic Newton–Lorentz equation. For a single particle the information contained in (19.114) and (19.115) for the Cartesian coordinates $i = x, y$, and z can be expressed in vectorial form as follows:

$$\dot{\mathbf{r}} = \nabla_{\mathbf{p}} H(\mathbf{r}, \mathbf{p}, t), \quad (19.151)$$

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{r}} H(\mathbf{r}, \mathbf{p}, t), \quad (19.152)$$

where $\nabla_{\mathbf{p}}$ and $\nabla_{\mathbf{r}}$ denote the gradient operators in $\mathbf{p}$ - and $\mathbf{r}$ -space. By combining (19.150) and (19.151) one obtains the relation in (11.81) between the kinematical (mechanical) and canonical momenta. Differentiation of this equation with respect to time, and subsequent use of (19.152) next give

$$m \frac{d^2}{dt^2} \mathbf{r}(t) = -\nabla_{\mathbf{r}} H(\mathbf{r}(t), \mathbf{p}(t), t) - q \frac{d}{dt} \mathbf{A}(\mathbf{r}(t), t). \quad (19.153)$$

Above it has been stressed that the position and momentum of the particle are functions of time. This for instance implies that

$$\frac{d}{dt} \mathbf{A}(\mathbf{r}(t), t) = \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} \mathbf{A}(\mathbf{r}, t) + \frac{\partial}{\partial t} \mathbf{A}(\mathbf{r}, t). \quad (19.154)$$

Keeping this in mind the reader may verify that (19.153), with the Hamilton function in (19.150), as claimed leads to the Newton–Lorentz equation of motion

$$m\ddot{\mathbf{r}} = q \left[-\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi + \dot{\mathbf{r}} \times (\nabla \times \mathbf{A}) \right] = q (\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (19.155)$$

In the special case where the scalar and vector potentials (to a good approximation) are time independent, and the electric and magnetic fields thus are static, Hamilton's characteristic function

$$W_0(\mathbf{r}) = S_0(\mathbf{r}, t) + Et \quad (19.156)$$

satisfies the equation

$$(\nabla W_0(\mathbf{r}) - q\mathbf{A}(\mathbf{r})) \cdot (\nabla W_0(\mathbf{r}) - q\mathbf{A}(\mathbf{r})) = 2m(E - q\phi(\mathbf{r})). \quad (19.157)$$

The surfaces of constant W_0 in configuration space have fixed locations whereas the surfaces of constant S_0 move. In a sense, these last surfaces thus may be considered as wave fronts propagating in configuration space. As a given S_0 wave front moves in time it will coincide with different constant- W_0 surfaces. It appears from (19.156) that the differential change in W_0 over the infinitesimal time interval dt is given by

$$dW_0 = E dt. \quad (19.158)$$

If ds denotes the local infinitesimal distance between neighboring W_0 surfaces one has

$$dW_0 = |\nabla W_0| ds. \quad (19.159)$$

Together, (19.158) and (19.159) show that the local speed of the S_0 wave front is given by

$$u = \frac{ds}{dt} = \frac{E}{|\nabla W_0|} = \frac{E}{|m\mathbf{v} + q\mathbf{A}(\mathbf{r})|}. \quad (19.160)$$

The local particle (v) and wave front (u) speeds hence are not the same. The unphysical character of the wave fronts in classical particle mechanics also manifests itself by the fact that u is gauge dependent in general. If the vector potential vanishes one obtains the simple relation

$$uv = \frac{E}{m} \quad (19.161)$$

between the speeds, and the equation for Hamilton's characteristic function takes the following form:

$$\nabla W_0(\mathbf{r}) \cdot \nabla W_0(\mathbf{r}) = 2m(E - q\phi(\mathbf{r})). \quad (19.162)$$

This last equation is form-identical to the eikonal equation in geometrical optics ((19.28) for a real refractive index, or equivalently (19.42)).

19.5.2 Quantum Potential and Probability Fluid Flow

Let us now return to the quantum mechanical Hamilton–Jacobi equation in (19.146). The presence of the quantum term (right-hand side of the equation) implies that the eikonal is a complex quantity, i.e.,

$$S(\mathbf{r}, t) = S_R(\mathbf{r}, t) + iS_I(\mathbf{r}, t). \quad (19.163)$$

By using this division, one obtains from the real and imaginary parts of (19.146) the following coupled equations between S_R and S_I :

$$\frac{1}{2m} (\nabla S_R - q\mathbf{A}) \cdot (\nabla S_R - q\mathbf{A}) + q\phi + \frac{\partial S_R}{\partial t} = \frac{1}{2m} (\nabla S_I \cdot \nabla S_I - \hbar \nabla^2 S_I), \quad (19.164)$$

$$\frac{1}{m} (\nabla S_R - q\mathbf{A}) \cdot \nabla S_I + \frac{\partial S_I}{\partial t} = \frac{\hbar}{2m} \nabla \cdot (\nabla S_R - q\mathbf{A}). \quad (19.165)$$

Since,

$$\hbar^2 \nabla^2 \exp\left(-\frac{S_I}{\hbar}\right) = (\nabla S_I \cdot \nabla S_I - \hbar \nabla^2 S_I) \exp\left(-\frac{S_I}{\hbar}\right), \quad (19.166)$$

Equation (19.164) can be written in the form

$$\frac{\partial S_R}{\partial t} + \frac{1}{2m} (\nabla S_R - q\mathbf{A})^2 + q\phi - \frac{\hbar^2}{2m} \frac{\nabla^2 \exp\left(-\frac{S_I}{\hbar}\right)}{\exp\left(-\frac{S_I}{\hbar}\right)} = 0. \quad (19.167)$$

By a comparison to (19.148) it is tempting to think of (19.167) as a kind of “classical” Hamilton–Jacobi equation, provided the last term is considered as a scalar potential energy (“quantum potential energy” [262, 263]) that must be added to the conventional potential energy, $q\phi(\mathbf{r}, t)$. The exponential function appearing in the quantum potential is proportional to the square root of the charge probability density, which is given by

$$\rho(\mathbf{r}, t) = q|\psi(\mathbf{r}, t)|^2 = q|\psi_0|^2 \exp\left(-\frac{2}{\hbar} S_I(\mathbf{r}, t)\right). \quad (19.168)$$

In the classical limit ($\hbar \rightarrow 0$), (19.167) is reduced to the Hamilton–Jacobi equation in (19.148).

Let us finally show that (19.165) in a sense has a simple physical interpretation. With the ansatz in (19.145) for the wave function, and the division in (19.163) of the eikonal, it is not difficult to prove that the probability current density in (11.125) is given by

$$\mathbf{J}(\mathbf{r}, t) = \frac{\rho}{m} (\nabla S_R - q\mathbf{A}), \quad (19.169)$$

and its divergence by

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) = \frac{\rho}{m} \left(\nabla - \frac{2}{\hbar} \nabla S_I \right) \cdot (\nabla S_R - q\mathbf{A}). \quad (19.170)$$

Since

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) = -\frac{2}{\hbar} \rho \frac{\partial S_I}{\partial t}, \quad (19.171)$$

the results in (19.170) and (19.171) show that the equation of continuity for the charge probability density (19.124) can be written in the form

$$\frac{\rho}{m} \left[\left(\nabla - \frac{2}{\hbar} \nabla S_I \right) \cdot (\nabla S_R - q\mathbf{A}) - \frac{2m}{\hbar} \frac{\partial S_I}{\partial t} \right] = 0. \quad (19.172)$$

Since ρ is not identically zero, the factor to ρ/m in (19.172) must vanish. A simple rearrangement shows that this demand is precisely what (19.165) expresses. The continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left[\rho \frac{\nabla S_R - q\mathbf{A}}{m} \right] = 0 \quad (19.173)$$

in a sense states that the charge probability is like a fluid that flows with a velocity

$$\mathbf{v}_{\text{fluid}} = m^{-1} (\nabla S_R - q\mathbf{A}). \quad (19.174)$$

Since $\nabla \times \mathbf{v}_{\text{fluid}} = -(q/m)\mathbf{B}$, the flow is irrotational when no magnetic field is present. In David Bohm's interpretation of quantum mechanics, (19.167) and (19.173) play a conceptually important role.

19.5.3 Relativistic Hamilton–Jacobi Equation: Particle of Zero Spin

We shall begin this brief study of the eikonal description in relativistic quantum mechanics with a derivation of the relativistic classical eikonal equation. The explicit expression for the classical standard Hamiltonian for a system of charged spinless particles interacting via the electromagnetic field was given in Sect. 11.4.1, (11.86). As a reminder of the final steps in the derivation of (11.86), let us repeat these assuming that we have only a single particle in the field. In this case one obtains from (11.84) and (11.85)

$$H = \gamma m c_0^2 + q\phi, \quad (19.175)$$

where m is the particle's rest mass. As it stands, H depends on the speed (v) of the particle through $\gamma = [1 - (v/c_0)^2]^{-1/2}$. It is easy, however, to eliminate γ in favor of an expression containing the canonical momentum. Thus, by squaring the relativistic connection

$$\gamma m \mathbf{v} = \mathbf{p} - q \mathbf{A}, \quad (19.176)$$

one obtains after a few elementary calculations

$$\gamma = \left[1 + \left(\frac{\mathbf{p} - q \mathbf{A}}{mc_0} \right)^2 \right]^{1/2}, \quad (19.177)$$

and hence

$$H = c_0 \left[(mc_0)^2 + (\mathbf{p} - q \mathbf{A})^2 \right]^{1/2} + q\phi, \quad (19.178)$$

in agreement with the result in (11.86). The Hamilton–Jacobi equation for Hamilton's principal function S (19.140) consequently takes the relativistic form

$$c_0 \left[(mc_0)^2 + (\nabla S - q \mathbf{A})^2 \right]^{1/2} + q\phi + \frac{\partial S}{\partial t} = 0. \quad (19.179)$$

As it soon will become clear it is useful to square this equation. This gives

$$c_0^2 (\nabla S - q \mathbf{A})^2 + (mc_0^2)^2 = \left(\frac{\partial S}{\partial t} + q\phi \right)^2, \quad (19.180)$$

and all solutions to (19.179) will also be solutions to (19.180).

A relativistic generalization of the Schrödinger equation is suggested by the usual heuristic procedure. Starting from the squared relativistic energy–momentum relation

$$E^2 = (pc_0)^2 + (mc_0^2)^2 \quad (19.181)$$

for a free particle, and letting the corresponding operator equation [$E \Rightarrow i\hbar\partial/\partial t$, $\mathbf{p} \Rightarrow (\hbar/i)\nabla$] act on the wave function $\psi(\mathbf{r}, t)$ one finds the so-called Klein–Gordon equation

$$\left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) \psi(\mathbf{r}, t) = q_C^2 \psi(\mathbf{r}, t), \quad (19.182)$$

where $q_C = mc_0/\hbar$ is the Compton wave number of the particle. The Klein–Gordon equation describes particles of zero spin. It should be mentioned here that the equation originally was obtained by Schrödinger, and this even before he wrote down his nonrelativistic version. The vectorial wave function of a massive transverse photon, $\mathbf{a}_T^{(+)}(\mathbf{r}, t)$, satisfies the wave equation in (19.55). This equation is of course satisfied not only by the analytical part of $\mathbf{a}_T(\mathbf{r}, t)$, but also by $\mathbf{a}_T(\mathbf{r}, t)$ itself, i.e.,

$$\left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) \mathbf{a}_T(\mathbf{r}, t) = Q_C^2 \mathbf{a}_T(\mathbf{r}, t). \quad (19.183)$$

At this point the reader should notice the form-identity of the Klein–Gordon equation and (19.183). Both can describe particles ($E > 0$) and antiparticles ($E < 0$). The vectorial wave function $\mathbf{a}_T(\mathbf{r}, t)$ relates to spin-one particles (antiparticles), here massive transverse photons, and the scalar $\psi(\mathbf{r}, t)$ to spin-zero particles (antiparticles).

The Klein–Gordon equation for a (charged) particle in an electromagnetic field is established starting from the covariant form of (19.182). Upon multiplication with $(\hbar/i)^2$ the equation becomes

$$[\hat{p}_\mu \hat{p}^\mu + (mc_0)^2] \psi = 0, \quad (19.184)$$

where $\hat{p}_\mu = (\hbar/i)\partial_\mu$. The minimal coupling replacements

$$\hat{p}_\mu \Rightarrow \hat{p}_\mu - qA_\mu, \quad \mu = 0, 1, 2, 3, \quad (19.185)$$

which in elementary notation read

$$\hat{\mathbf{p}} \Rightarrow \frac{\hbar}{i} \nabla - q\mathbf{A}, \quad (19.186)$$

$$\hat{p}_0 \Rightarrow \frac{1}{c_0} \left(\frac{\hbar}{i} \frac{\partial}{\partial t} + q\phi \right), \quad \hat{p}^0 = -\hat{p}_0, \quad (19.187)$$

transfer the coupled covariant Klein–Gordon equation

$$[(\hat{p}_\mu - qA_\mu)(\hat{p}^\mu - qA^\mu) + (mc_0)^2] \psi = 0 \quad (19.188)$$

to the form

$$c_0^2 \left[\left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right)^2 + (mc_0)^2 \right] \psi(\mathbf{r}, t) = \left(\frac{\hbar}{i} \frac{\partial}{\partial t} + q\phi \right)^2 \psi(\mathbf{r}, t). \quad (19.189)$$

By inserting the eikonal ansatz given in (19.145) into (19.189) the reader may show that the eikonal satisfies the partial differential equation

$$\begin{aligned} & (\nabla S - q\mathbf{A})^2 + (mc_0)^2 - \frac{1}{c_0^2} \left(\frac{\partial S}{\partial t} + q\phi \right)^2 \\ &= i\hbar \left[\left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) S - q \left(\nabla \cdot \mathbf{A} + \frac{1}{c_0^2} \frac{\partial \phi}{\partial t} \right) \right]. \end{aligned} \quad (19.190)$$

This equation, apparently not often written down in the literature, may be called the relativistic quantum mechanical Hamilton–Jacobi equation for a spinless particle.

In the Lorenz gauge the equation takes the simpler form

$$(\nabla S - q\mathbf{A})^2 + (mc_0)^2 - \frac{1}{c_0^2} \left(\frac{\partial S}{\partial t} + q\phi \right)^2 = i\hbar \left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) S, \quad (19.191)$$

and in the classical limit ($\hbar \rightarrow 0$), it reduces precisely to (19.180), which we know is equivalent to the relativistic Newton–Lorentz equation of motion. It is possible to show that the quantum mechanical eikonal equation for the minimally coupled Dirac equation, which describes relativistic spin one-half particles (anti-particles), reduces to the classical relativistic eikonal equation for a spinless particle, i.e., (19.180). Since the spin concept does not exist for a classical point particle this result is perhaps not surprising. It may finally be noticed that the relativistic eikonal equation in manifestly covariant notation reads

$$(\partial_\mu S - qA_\mu) (\partial^\mu S - qA^\mu) + (mc_0)^2 = i\hbar \partial_\mu (\partial^\mu S - qA^\mu), \quad (19.192)$$

as one readily realizes from (19.190).

Chapter 20

Spin-1/2 Currents: Spatial Photon Localization in Emission from a Pure Spin Transition

It appears from the analyses in Chaps. 14 and 18 that in a photon emission process from a charged-particle source, described by the microscopic current density distribution $\mathbf{J}(\mathbf{r}, t)$, the transverse photon embryo is never better confined in space than the extension of the transverse current density ($\mathbf{J}_T(\mathbf{r}, t)$) domain. This best confinement only appears in the very first instance of the emission process, and it is not selfcontradictory to consider the $\mathbf{J}_T(\mathbf{r}, t)$ domain as the source region of the transverse photon. In general, the rim zone must therefore be included as a part of the source domain, and we have seen that the volume of this zone is much larger than the electronic volume of the micro- or mesoscopic object emitting the photon. *If* one could meet the condition $\mathbf{J}_T(\mathbf{r}, t) = \mathbf{J}(\mathbf{r}, t)$ it would be possible to achieve a much stronger spatial confinement of the transverse photon embryo in the initial phase of the emission process from a mesoscopic (or microscopic) particle. In the present chapter, we shall realize that the photon emissions from pure spin transitions meet the above mentioned requirement. When $\mathbf{J}_T(\mathbf{r}, t) = \mathbf{J}(\mathbf{r}, t)$, I call the transverse photon source super-confined, and the initial embryo state may be characterized as super-localized.

20.1 Spin-1/2 Current Density

As a first step towards a space–time description of the photon emission from a spin transition we shall derive an expression for the spin contribution to the quantum mechanical probability current density of a spin-1/2 particle (electron). Since the spin is a relativistic concept we start from the Dirac equation, treated here as a one-particle relativistic wave equation. After having established the appropriate formulas for the Dirac charge and current density probabilities we find an expression for the current density in the weakly relativistic regime. A part of this expression gives us the spin contribution to the quantum mechanical current density in the framework of the two-component Pauli theory. The associated spin-1/2 current density operator is the starting point for the subsequent study of the transverse photon emission from pure spin transitions.

20.1.1 Dirac Equation in Minimal Coupling Form

Let us begin with a very brief review of the Dirac wave equation in its unquantized form. The nonrelativistic Schrödinger equation for a free particle can be obtained heuristically from the energy–momentum relation $E = p^2/(2m)$ if one first replace E and $\mathbf{p}$ by the quantum mechanical operators

$$\hat{E} = i\hbar \frac{\partial}{\partial t}, \quad (20.1)$$

$$\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla, \quad (20.2)$$

and then let the corresponding operator equation act on the wave function $\psi(\mathbf{r}, t)$. A relativistic generalization of the Schrödinger equation in which space and time enter in a symmetric manner, and which is a first-order partial differential equation, can be obtained starting from a linear relation between E and $\mathbf{p}$ which also contains a term proportional to the rest mass energy. Thus, one sets

$$E = c_0 \boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc_0^2, \quad (20.3)$$

where $\boldsymbol{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$ and β are real and dimensionless quantities. Since (20.3) must be compatible with the relativistic energy–momentum relation in (16.61) certain restrictions are put on $\boldsymbol{\alpha}$ and β , as we shall see now. The square of (20.3) is

$$E^2 = c_0 \sum_{i,j} \alpha_i \alpha_j p_i p_j + mc_0^3 \sum_i (\alpha_i \beta + \beta \alpha_i) p_i + m^2 c_0^4 \beta^2, \quad (20.4)$$

where $i, j = x, y, z$. A comparison of (16.61) and (20.4) leads to the following relations:

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij}, \quad (20.5)$$

$$\alpha_i \beta + \beta \alpha_i = 0, \quad (20.6)$$

$$\beta^2 = 1. \quad (20.7)$$

It is clear from (20.5)–(20.7) that β and the α_i 's cannot be simple numbers. One can find matrices, however, which satisfy these relations. Since, later on the right-hand side of (20.3) will be translated into a Hamilton operator (observable), the matrices representing the α_i 's and β must be Hermitian, and therefore square. For compactness, we shall in the following not write the β and α_i 's in boldface, as it has been the practice for matrices up to now in this book. It appears from (20.6) that α_i and β anticommute, and this implies that β and the α_i 's must be traceless. This can be seen as follows:

$$\text{Tr}\{\alpha_i\} = -\text{Tr}\{\beta \alpha_i \beta^{-1}\} = -\text{Tr}\{\beta^{-1} \beta \alpha_i\} = -\text{Tr}\{\alpha_i\}, \quad (20.8)$$

and, therefore,

$$\text{Tr}\{\alpha_i\} = 0, \quad i = x, y, z. \quad (20.9)$$

An analogous result for the trace of β , i.e.,

$$\text{Tr}\{\beta\} = 0, \quad (20.10)$$

also follows from (20.6), as the reader may verify. Since $\alpha_i^2 = \beta^2 = 1$, where 1 is the $N \times N$ unit matrix, the eigenvalues of α_i and β are ± 1 . To prove this let us consider the eigenvalue equation for (say) β , i.e., $\beta A = aA$, where A is an eigenvector of β and a the associated eigenvalue. Note that vectors are not written in boldface here and in the following. By acting on the eigenvalue equation by β from the left one obtains $\beta^2 A = \beta(aA) = a(\beta A) = a^2 A$, and since $\beta^2 = 1$ (20.7) one has $A = a^2 A$. The possible eigenvalues of β therefore are ± 1 as claimed. An analogous proof can be given for the α_i 's, of course. Since the trace of a matrix is the sum of the eigenvalues, the α_i 's and β must be of even dimensions. The identity matrix along with the three Pauli matrices (11.112) form a basis for the set of 2×2 matrices, as may easily be proved. For $N = 2$, only three anticommuting matrices – the Pauli matrices – therefore exist. The dimension of the α_i 's and β thus cannot be smaller than 4×4 (but certainly higher). The four Dirac matrices

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (20.11)$$

which are Hermitian, traceless, and have eigenvalues ± 1 form a possible realization of (20.5)–(20.7). The σ_i 's entering (20.11) are the Pauli matrices (11.112). The choice in (20.11) is not unique. All sets of matrices α'_i and β' related to these by $\alpha'_i = U\alpha_i U^{-1}$ and $\beta' = U\beta U^{-1}$, where U is an arbitrary 4×4 unitary matrix, are allowed as realizations of (20.5)–(20.7). The reader is prompted to prove this by herself.

The Dirac equation is obtained using the heuristic procedure sketched in the beginning of this subsection. For a free spin-1/2 particle one thus is led to the relativistic wave equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = (c_0 \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta mc_0^2) \psi(\mathbf{r}, t). \quad (20.12)$$

The rank $N = 4$ of the matrices entering (20.12) necessitates that the wave function $\psi(\mathbf{r}, t)$ is a spinor with four components. In turn, this implies the existence of certain internal degrees of freedom for the Dirac particle. The Dirac equation for a charged spin-1/2 particle in an electromagnetic field, described by the potentials $\mathbf{A}$ and φ , is obtained making the minimal coupling substitutions (already discussed in relation to the Klein–Gordon equation in Sect. 19.5.3)

$$i\hbar \frac{\partial}{\partial t} \Rightarrow i\hbar \frac{\partial}{\partial t} - q\phi(\mathbf{r}, t), \quad (20.13)$$

$$\frac{\hbar}{i} \nabla \Rightarrow \frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{r}, t), \quad (20.14)$$

in (20.12). The substitution rule is, as we know, related to the local phase invariance principle in quantum mechanics (Sect. 11.6.4). Thus, one finally arrives at the following relativistic wave equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \hat{H}_D \psi(\mathbf{r}, t), \quad (20.15)$$

where

$$\hat{H}_D = \beta mc_0^2 + c_0 \boldsymbol{\alpha} \cdot \left(\frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{r}, t) \right) + 1 q\phi(\mathbf{r}, t) \quad (20.16)$$

is the Dirac (D) Hamilton operator. By means of the symbol 1 it has been stressed that the term containing the scalar potential in $\hat{H}_D$ is proportional to the unit matrix (1).

20.1.2 Fully Relativistic Dirac Current Density

On the basis of the Dirac equation in (20.15) we now shall establish a certain relation which one may interpret as a quantum mechanical equation of continuity for the charge. Let $\psi^\dagger \equiv \psi^*$ be the Hermitian conjugate row vector (spinor) of ψ [$\sim$ stands for transposing]. By multiplying the Dirac equation with $\psi^\dagger$ from the left one obtains the scalar relation.

$$i\hbar \psi^\dagger \frac{\partial \psi}{\partial t} = c_0 \psi^\dagger \boldsymbol{\alpha} \cdot \left(\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \psi + q\phi \psi^\dagger \psi + mc_0^2 \psi^\dagger \beta \psi. \quad (20.17)$$

Forming the Hermitian conjugate of the Dirac equation and multiplying this by ψ from the right gives

$$-i\hbar \left(\frac{\partial \psi^\dagger}{\partial t} \right) \psi = c_0 \left(-\frac{\hbar}{i} \nabla - q\mathbf{A} \right) \cdot (\psi^\dagger \boldsymbol{\alpha}) \psi + q\phi \psi^\dagger \psi + mc_0^2 \psi^\dagger \beta \psi, \quad (20.18)$$

since $\alpha_i^\dagger = \alpha_i$ and $\beta_i^\dagger = \beta_i$. By subtracting (20.18) from (20.17) one obtains after a few calculations

$$i\hbar \frac{\partial}{\partial t} (\psi^\dagger \psi) = c_0 \frac{\hbar}{i} \nabla \cdot (\psi^\dagger \boldsymbol{\alpha} \psi). \quad (20.19)$$

It appears obvious now to write the result above in the form

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \frac{\partial}{\partial t} \rho(\mathbf{r}, t) = 0, \quad (20.20)$$

where

$$\rho(\mathbf{r}, t) = q\psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t), \quad (20.21)$$

and

$$\mathbf{J}(\mathbf{r}, t) = qc_0\psi^\dagger(\mathbf{r}, t)\boldsymbol{\alpha}\psi(\mathbf{r}, t). \quad (20.22)$$

At this point in the development one interprets $\rho(\mathbf{r}, t)$ and $\mathbf{J}(\mathbf{r}, t)$ as the charge and current probability densities in the one-particle relativistic wave equation. With this interpretation (20.20) is just the equation of continuity for the charge in relativistic quantum mechanics. It follows from the equation of continuity that $(c_0\rho, \mathbf{J})$ forms a four-vector under Lorentz transformations. This can also be shown by a direct calculation. It is remarkable that the vector potential does not appear explicitly in the expression for the relativistic current density, as it does in the nonrelativistic limit; see (11.126)–(11.128). The form of (20.22) suggests that the *operator* (operator symbol $\wedge$ reinserted)

$$\hat{\mathbf{v}} \equiv c_0\hat{\boldsymbol{\alpha}} \quad (20.23)$$

serves as a relativistic velocity operator in the Dirac theory. It appears from the analysis between (20.10) and (20.11) that the eigenvalues of the mutually noncommuting components $c_0\hat{\alpha}_i$ ($i = x, y, z$) of $\hat{\mathbf{v}}$ are $\pm c_0$. At first sight this is a surprising result, since it suggests that a massive spin-1/2 particle can move with the speed of light in the framework of relativistic quantum mechanics. A more refined analysis shows that this result is *not* in conflict with the special theory of relativity, due to the fact that the $\mathbf{r}$ -operator in the relativistic theory must be interpreted as a kind of mean position operator, the mean being over a volume which linear extension is of the order of the Compton wavelength of the particle [250]. Perhaps this conclusion is not so surprising after all because relativistic quantum mechanics must be replaced by its covering theory, relativistic quantum field theory, once lengths qualitatively comparable to or smaller than the Compton wavelength play a role.

20.1.3 Weakly Relativistic Pauli Spin Current Density

We have seen that the relativistic wave function of a spin-1/2 particle can be represented as a four-component spinor

$$\psi(\mathbf{r}, t) = \begin{pmatrix} \psi_1(\mathbf{r}, t) \\ \psi_2(\mathbf{r}, t) \\ \psi_3(\mathbf{r}, t) \\ \psi_4(\mathbf{r}, t) \end{pmatrix}, \quad (20.24)$$

and the Dirac equation in (20.15) therefore appears as a set of coupled differential equations among the ψ_i 's [$i = 1 - 4$]. The special block structures of the α_i and β matrices (20.11) make it possible to write the set in the form of two coupled equations among the two-component spinors

$$\phi(\mathbf{r}, t) \equiv \begin{pmatrix} \psi_1(\mathbf{r}, t) \\ \psi_2(\mathbf{r}, t) \end{pmatrix}, \quad \chi(\mathbf{r}, t) \equiv \begin{pmatrix} \psi_3(\mathbf{r}, t) \\ \psi_4(\mathbf{r}, t) \end{pmatrix}. \quad (20.25)$$

When $\psi(\mathbf{r}, t)$ is represented by a pair of two-component spinors, i.e.,

$$\psi(\mathbf{r}, t) = \begin{pmatrix} \phi(\mathbf{r}, t) \\ \chi(\mathbf{r}, t) \end{pmatrix} \quad (20.26)$$

it is often called a bispinor. In bispinor notation, the Dirac equation gives the two coupled wave equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = c_0 \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A}) \begin{pmatrix} \chi \\ \phi \end{pmatrix} + qc_0 A^0 \begin{pmatrix} \phi \\ \chi \end{pmatrix} + mc_0^2 \begin{pmatrix} \phi \\ -\chi \end{pmatrix}. \quad (20.27)$$

A slight reduction of the coupling problem is obtained by substitution of the ansatz

$$\begin{pmatrix} \phi(\mathbf{r}, t) \\ \chi(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} \phi_0(\mathbf{r}, t) \\ \chi_0(\mathbf{r}, t) \end{pmatrix} \exp\left(-i \frac{mc_0^2 t}{\hbar}\right) \quad (20.28)$$

into the Dirac equation in (20.27). This ansatz is of particular importance for low energy studies where the rest energy mc_0^2 is much larger than all other relevant energies. At low energies the functions $\phi_0(\mathbf{r}, t)$ and $\chi_0(\mathbf{r}, t)$ are slowly varying functions of time in comparison to the exponential function in (20.28). Independent of the magnitude of the particle energy these functions satisfy the set of equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \phi_0 \\ \chi_0 \end{pmatrix} = c_0 \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A}) \begin{pmatrix} \chi_0 \\ \phi_0 \end{pmatrix} + qc_0 A^0 \begin{pmatrix} \phi_0 \\ \chi_0 \end{pmatrix} - 2mc_0^2 \begin{pmatrix} 0 \\ \chi_0 \end{pmatrix}. \quad (20.29)$$

If the kinetic energy of the particle and the electrostatic potential energy are small in comparison to the rest energy it is reasonable to assume that

$$\left| i\hbar \frac{\partial \chi_0}{\partial t} \right|, |qc_0 A^0 \chi_0| \ll |mc_0^2 \chi_0|. \quad (20.30)$$

With these approximations, the lower component of (20.29) gives to lowest order

$$\chi_0 = \frac{1}{2mc_0} \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A}) \phi_0. \quad (20.31)$$

In the so-called weakly relativistic domain (characterized by (20.31)), χ_0 thus is a factor of the order v/c_0 less than ϕ_0 . With this in mind, χ_0 and ϕ_0 are often referred to as the small and large components of ψ . The approximation in (20.31) is sufficient for the study that follows of the spin current density. By inserting (20.31) into the upper component of (20.29), the following quantum mechanical wave equation is obtained for the two-component spinor ϕ_0 :

$$i\hbar \frac{\partial \phi_0}{\partial t} = \frac{1}{2m} [\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})] [\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})] \phi_0 + qc_0 A^0 \phi_0. \quad (20.32)$$

As we now shall demonstrate, the Dirac equation in (20.32) for the large component ϕ_0 is identical to the two-component Pauli equation for a spin-1/2 particle written in its standard form. This form is reached by means of the identity

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} 1 + i \boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}), \quad (20.33)$$

where $\mathbf{a}$ and $\mathbf{b}$ are two arbitrary vectors, or vector operators, whose three components commute with all operators acting in the two-dimensional spin state space. Note that if $\mathbf{a}$ and $\mathbf{b}$ do not commute they must appear in the order shown. By utilizing the formula for spin products given in (11.113) the reader may prove the correctness of (20.33). With $\mathbf{a} = \mathbf{b} = \hat{\mathbf{p}} - q\mathbf{A}$, one finds

$$[\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})] [\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A})] = (\hat{\mathbf{p}} - q\mathbf{A})^2 - q\hbar \boldsymbol{\sigma} \cdot \nabla \times \mathbf{A}. \quad (20.34)$$

In obtaining this result we have used the vector identity

$$\nabla \times (\mathbf{A} \phi_0) = (\nabla \times \mathbf{A}) \phi_0 - \mathbf{A} \times \nabla \phi_0. \quad (20.35)$$

For brevity, also the unit matrix (1) has been omitted in the notation for the first term on the right side of (20.34). By inserting the relation in (20.34) into (20.32) one finally gets the following wave equation for the large component:

$$i\hbar \frac{\partial \phi_0}{\partial t} = \left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + qc_0 A^0 - \frac{q\hbar}{2m} \boldsymbol{\sigma} \cdot \nabla \times \mathbf{A} \right] \phi_0. \quad (20.36)$$

This quantum mechanical two-component wave equation is precisely the Pauli equation for a spin-1/2 particle in an electromagnetic field described by the four-potential $\{A^\mu\} = (A^0 = \phi/c_0, \mathbf{A})$. The Hamilton operator in (20.36) agrees with the single-particle version of (11.111) for a gyromagnetic factor $g = 2$.

Let us now turn our attention towards the calculation of the spin-1/2 probability current density in the weakly relativistic limit. On the basis of the realization given

for the α_i 's in (20.11), and the bispinor notation in (20.28), it is obvious that the Dirac current density (20.22) can be written in the form

$$\mathbf{J}(\mathbf{r}, t) = c_0 q \left[\psi_0^\dagger \boldsymbol{\sigma} \chi_0 + \chi_0^\dagger \boldsymbol{\sigma} \psi_0 \right], \quad (20.37)$$

where the last term in the parenthesis is the Hermitian conjugate of the first term, since $\sigma_i = \sigma_i^\dagger$, for all i . It is perhaps not unexpected that the rest mass energy does not appear explicitly in (20.37). By utilizing the approximation in (20.31) it appears that the current density in the weakly relativistic domain is given by

$$\mathbf{J}(\mathbf{r}, t) = \frac{q}{2m} \left[\phi_0^\dagger \boldsymbol{\sigma} \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A}) \phi_0 + h.c. \right]. \quad (20.38)$$

The current density in (20.38) can be divided into so-called space and spin parts with the help of the easily proved identity

$$\boldsymbol{\sigma} \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} - q\mathbf{A}) = 1 (\hat{\mathbf{p}} - q\mathbf{A}) - i \boldsymbol{\sigma} \times (\hat{\mathbf{p}} - q\mathbf{A}). \quad (20.39)$$

Thus,

$$\mathbf{J}(\mathbf{r}, t) = \mathbf{J}^{\text{space}}(\mathbf{r}, t) + \mathbf{J}^{\text{spin}}(\mathbf{r}, t), \quad (20.40)$$

where (omitting again writing the unit matrix between the two-component spinors)

$$\mathbf{J}^{\text{space}}(\mathbf{r}, t) = \frac{q}{2m} \left[\phi_0^\dagger (\hat{\mathbf{p}} - q\mathbf{A}) \phi_0 + h.c. \right], \quad (20.41)$$

and tentatively

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \frac{q}{2m} \left[i \phi_0^\dagger (\hat{\mathbf{p}} - q\mathbf{A}) \times \boldsymbol{\sigma} \phi_0 + h.c. \right]. \quad (20.42)$$

Since the Pauli spin matrices are Hermitian [$\boldsymbol{\sigma} = \boldsymbol{\sigma}^\dagger$] the two terms containing the factor $q\mathbf{A}$ in (20.42) cancel each other, and the spin current density hence takes the simpler form

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \frac{iq}{2m} \phi_0^\dagger \hat{\mathbf{p}} \times \boldsymbol{\sigma} \phi_0 + h.c. \quad (20.43)$$

The result in (20.43) is the basic one for the following discussion of the photon localization and emission from pure spin transitions. Before ending this subsection it should be emphasized that although the expression in (20.43) for $\mathbf{J}^{\text{spin}}$ does not depend explicitly on the small component of the Dirac wave function this component cannot be set to zero from the outset, because the relation in (20.31) between χ_0 and ϕ_0 was used in the determination of the weakly relativistic spin current density. In the hole theory, proposed by Dirac to deal with the negative-energy states of his relativistic wave equation, the particle–antiparticle (electron–positron) concept emerges. In relation to the present calculation of the spin current density this

means that the Pauli spin-1/2 concept is rooted in the particle–antiparticle coupling. In a sense it is the indirect presence of the antiparticle (positron) in the weakly relativistic theory which sets the limit for the spatial localization of the particle (electron). It is also the particle–antiparticle coupling which is responsible for the fact that the $\mathbf{r}$ -operator, as mentioned earlier, must be interpreted as a sort of mean position operator.

20.2 Spin Source for Photons: Absence of the Rim Zone

For what follows it is convenient to expand the quantum state $|\phi_0\rangle$ of the weakly relativistic spin-1/2 particle in the $\mathbf{r}$ -representation and the (S^2, S_z) -spin basis. Hence, the two-component Pauli spinor is

$$\phi_0(\mathbf{r}, t) = \begin{pmatrix} \langle \mathbf{r}; \uparrow | \phi_0 \rangle \\ \langle \mathbf{r}; \downarrow | \phi_0 \rangle \end{pmatrix} \equiv \begin{pmatrix} \psi_\uparrow(\mathbf{r}, t) \\ \psi_\downarrow(\mathbf{r}, t) \end{pmatrix}, \quad (20.44)$$

where $\psi_\uparrow(\mathbf{r}, t)$ and $\psi_\downarrow(\mathbf{r}, t)$ are the spin-up ($\uparrow$) and spin-down ($\downarrow$) components of the spinor. The Hermitian conjugate of $\phi_0(\mathbf{r}, t)$ is the row spinor $\phi_0^\dagger = (\psi_\uparrow^*, \psi_\downarrow^*)$. The spin probability current density in (20.43) also appears as the quantum mechanical mean value,

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \phi_0^\dagger(\mathbf{r}_e, t) \hat{\mathbf{J}}^{\text{spin}}(\mathbf{r}; \mathbf{r}_e) \phi_0(\mathbf{r}_e, t) d^3 r_e, \quad (20.45)$$

of the one-particle spin current density operator

$$\hat{\mathbf{J}}^{\text{spin}}(\mathbf{r}; \mathbf{r}_e) = \frac{iq}{2m} [\delta(\mathbf{r} - \mathbf{r}_e) \hat{\mathbf{p}}_e \times \boldsymbol{\sigma} - \hat{\mathbf{p}}_e \times \boldsymbol{\sigma} \delta(\mathbf{r} - \mathbf{r}_e)]. \quad (20.46)$$

The integration in (20.45) is over the particle (electron) coordinates, $\mathbf{r}_e$, and $\hat{\mathbf{p}}_e = (\hbar/i) \nabla_e$. In order to express $\mathbf{J}^{\text{spin}}(\mathbf{r}, t)$ explicitly in terms of the spin-up and down wave functions, one notes that the operator

$$\boldsymbol{\sigma} \times \nabla = \begin{pmatrix} \hat{y} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial y} & \hat{z} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial z} + i \left(\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right) \\ \hat{z} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial z} - i \left(\hat{z} \frac{\partial}{\partial x} - \hat{x} \frac{\partial}{\partial z} \right) & \hat{x} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial x} \end{pmatrix} \quad (20.47)$$

may be written in the form

$$\boldsymbol{\sigma} \times \nabla = \begin{pmatrix} \hat{z} \times \nabla & \sqrt{2} \hat{\mathbf{e}}_- \times \nabla \\ \sqrt{2} \hat{\mathbf{e}}_+ \times \nabla & -\hat{z} \times \nabla \end{pmatrix}, \quad (20.48)$$

where $\hat{e}_{\pm} = (\hat{x} \pm i\hat{y})/\sqrt{2}$ are specific helicity unit vectors. By combining (20.43), (20.44) and (20.48) one finds

$$\begin{aligned} \mathbf{J}^{\text{spin}}(\mathbf{r}, t) = & \frac{q\hbar}{2m} \left[\hat{z} \times \nabla (|\psi_{\downarrow}(\mathbf{r}, t)|^2 - |\psi_{\uparrow}(\mathbf{r}, t)|^2) \right. \\ & \left. - \sqrt{2}\hat{e}_{+} \times \nabla (\psi_{\uparrow}(\mathbf{r}, t)\psi_{\downarrow}^{*}(\mathbf{r}, t)) - \sqrt{2}\hat{e}_{-} \times \nabla (\psi_{\downarrow}(\mathbf{r}, t)\psi_{\uparrow}^{*}(\mathbf{r}, t)) \right]. \end{aligned} \quad (20.49)$$

In the Pauli spinor formalism, the so-called space part of the one-particle current density (20.41) is given by

$$\mathbf{J}^{\text{space}}(\mathbf{r}, t) = \mathbf{J}_{\uparrow}^{\text{space}}(\mathbf{r}, t) + \mathbf{J}_{\downarrow}^{\text{space}}(\mathbf{r}, t), \quad (20.50)$$

where

$$\begin{aligned} \mathbf{J}_{\uparrow(\downarrow)}^{\text{space}}(\mathbf{r}, t) = & \frac{q\hbar}{2im} \left[\psi_{\uparrow(\downarrow)}^{*}(\mathbf{r}, t) \nabla \psi_{\uparrow(\downarrow)}(\mathbf{r}, t) - \psi_{\uparrow(\downarrow)}(\mathbf{r}, t) \nabla \psi_{\uparrow(\downarrow)}^{*}(\mathbf{r}, t) \right] \\ & - \frac{q^2}{m} |\psi_{\uparrow(\downarrow)}(\mathbf{r}, t)|^2 \mathbf{A}(\mathbf{r}, t). \end{aligned} \quad (20.51)$$

As one perhaps would expect, the space part of the quantum mechanical current density is the sum of pure spin-up and spin-down parts. Each of the two form-identical contributions consists of a paramagnetic part and a part which explicit dependence on the vector potential is linear. The result in (20.51) is in agreement with the result given in (11.126)–(11.128) for a nonrelativistic, and thus spinless, particle.

With the help of the vector identity $\nabla \cdot (\mathbf{V} \times \nabla v(\mathbf{r})) = 0$, which holds for a constant ($\mathbf{r}$ independent) vector $\mathbf{V}$, one immediately finds from (20.49) that

$$\nabla \cdot \mathbf{J}^{\text{spin}}(\mathbf{r}, t) = 0. \quad (20.52)$$

This result shows that the Pauli spin current density is a transverse vector field, i.e.,

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \mathbf{J}_{\text{T}}^{\text{spin}}(\mathbf{r}, t). \quad (20.53)$$

Physically this means that a spin current density distribution has no rim zone. In consequence, a photon emitted from a pure spin transition would have its source confined to the domain in which the particle (electron) probability density is non-vanishing. A schematic illustration of the source confinement, etc., is shown in Fig. 20.1. For an atom, or a mesoscopic particle, this in turn implies that the photon embryo would exhibit exponential spatial confinement in the initial phase of the emission process. Exponential confinement cannot be achieved unless the space part of the Pauli current density (20.50) vanishes. It appears from the equation of continuity (20.20) that this only can happen if the Pauli charge probability density

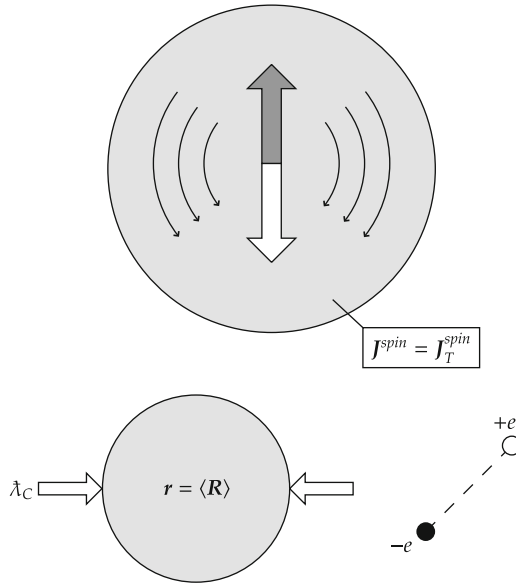


Fig. 20.1 Schematic illustration of the source confinement problem for a transverse photon emitted in a pure spin transition. *Top figure:* In a spin-flip a current is flowing in direct space around the point-particle, but since the flow is incompressible no rim zone exists, i.e., $\mathbf{J}_T^{\text{spin}} = \mathbf{J}^{\text{spin}}$. The photon source thus is confined to a region identical to the electronic size of the atom (or mesoscopic particle). *Bottom figure:* In relativistic quantum mechanics, even a spin source for photons cannot be truncated to a point, because the electron–positron coupling makes the $\mathbf{r}$ -vector in the Dirac equation a mean position vector, $\langle \mathbf{R} \rangle$, in a region of linear extension comparable to the Compton wavelength (divided by 2π), $\lambda_C = \hbar/(mc_0)$

$$\rho(\mathbf{r}, t) = \phi_0^\dagger(\mathbf{r}, t)\phi_0(\mathbf{r}, t) = q (|\psi_\uparrow(\mathbf{r}, t)|^2 + |\psi_\downarrow(\mathbf{r}, t)|^2) \quad (20.54)$$

becomes time independent. Such a demand is tantamount to the requirement that the spatial particle (electron) configuration does not change during the photon emission process. When the spatial dynamic freezes out, the state space for the state vector at all times is a simple tensor product of the space and spin state spaces. Thus, the Pauli spinor takes the form

$$\begin{pmatrix} \psi_\uparrow(\mathbf{r}, t) \\ \psi_\downarrow(\mathbf{r}, t) \end{pmatrix} = \psi(\mathbf{r}) \begin{pmatrix} \uparrow(t) \\ \downarrow(t) \end{pmatrix}, \quad (20.55)$$

where $\uparrow(t)$ and $\downarrow(t)$ are the spin-up and spin-down components of the spin wave function at the time t , and $\psi(\mathbf{r})$ is the relevant frozen spatial wave function. By inserting (20.55) into (20.49), the reader may verify that one obtains the following expression for the spin current density:

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \frac{q\hbar}{2m} \left\{ [|\downarrow(t)|^2 - |\uparrow(t)|^2] \hat{\mathbf{z}} - \sqrt{2} \uparrow(t) \downarrow^*(t) \hat{\mathbf{e}}_+ - \sqrt{2} \downarrow(t) \uparrow^*(t) \hat{\mathbf{e}}_- \right\} \times \nabla |\psi(\mathbf{r})|^2. \quad (20.56)$$

It appears from this result that *even* in a pure spin flip process a particle current flows in direct space in the domain where $|\psi(\mathbf{r}, t)|^2$ is nonvanishing for a fixed point-particle.

20.3 Photon Emission from Spin-1/2 Transitions

20.3.1 Electromagnetic Far Field

Since the Pauli spin current density is a transverse vector field we know that no longitudinal electric field accompanies spin-1/2 dynamics. In the space–frequency domain the transverse electric and magnetic fields generated by $\mathbf{J}_T^{\text{spin}}(\mathbf{r}; \omega) = \mathbf{J}^{\text{spin}}(\mathbf{r}'; \omega)$ are given by

$$\mathbf{E}_T(\mathbf{r}; \omega) = i\mu_0\omega \int_{-\infty}^{\infty} g(R; \omega) \mathbf{J}^{\text{spin}}(\mathbf{r}'; \omega) d^3r', \quad (20.57)$$

and

$$\mathbf{B}(\mathbf{r}; \omega) = \mu_0 \int_{-\infty}^{\infty} g(R; \omega) \nabla' \times \mathbf{J}^{\text{spin}}(\mathbf{r}'; \omega) d^3r'. \quad (20.58)$$

For what follows it is convenient to rewrite the integral expression for the magnetic field in the form

$$\mathbf{B}(\mathbf{r}; \omega) = \mu_0 \int_{-\infty}^{\infty} \nabla g(R; \omega) \times \mathbf{J}^{\text{spin}}(\mathbf{r}'; \omega) d^3r'. \quad (20.59)$$

The result above can be derived making some partial integrations in (20.58), and utilizing that $\nabla' g(R; \omega) = -\nabla g(R; \omega)$. Since $\mathbf{J}^{\text{spin}}(\mathbf{r}'; \omega)$ is nonzero only in a finite region of space, the surface integrals at infinity all vanish. If the particle in consideration is in a stationary state as far as the spatial degrees of freedom are concerned (time independent wave function: $\psi(\mathbf{r})$), the spin current density will in the space–time domain, as we have realized in the previous subsection, be given by

$$\mathbf{J}^{\text{spin}}(\mathbf{r}, t) = \boldsymbol{\alpha}(\mathbf{r}) \times \boldsymbol{\beta}(t), \quad (20.60)$$

where

$$\boldsymbol{\alpha}(\mathbf{r}) = \frac{q\hbar}{2m} \nabla |\psi(\mathbf{r})|^2, \quad (20.61)$$

and

$$\boldsymbol{\beta}(t) \equiv \langle \boldsymbol{\sigma} \rangle(t) = (\uparrow^*(t), \downarrow^*(t)) \boldsymbol{\sigma} \begin{pmatrix} \uparrow(t) \\ \downarrow(t) \end{pmatrix}. \quad (20.62)$$

As indicated in (20.62), $\boldsymbol{\beta}(t)$ is just the quantum mechanical mean value of the Pauli spin vector (operator). The Fourier transform of $\boldsymbol{\beta}(t)$ is denoted by $\boldsymbol{\beta}(\omega) = \langle \boldsymbol{\sigma} \rangle(\omega)$ below.

Let us assume that the spin source is located around the origo of the coordinate system. Far away from the source the emitted electromagnetic field takes a particularly simple form. Thus, when $|\mathbf{r}|$ is large enough, the approximation

$$|\mathbf{r} - \mathbf{r}'| \approx r - \hat{\mathbf{r}} \cdot \mathbf{r}' \quad (20.63)$$

can be used in the phases of the Huygens propagator, $g(R; \omega)$ and its gradient $\nabla g(R; \omega)$. Everywhere else, the simpler approximation $\mathbf{R} \approx \mathbf{r}$ ($|\mathbf{R}| = |\mathbf{r}|$) usually is sufficient. On using the approximations

$$g(R; \omega) \approx \frac{e^{iq_0 r}}{4\pi r} \exp(-iq_0 \hat{\mathbf{r}} \cdot \mathbf{r}'), \quad (20.64)$$

$$\nabla g(R; \omega) \approx \hat{\mathbf{r}} \frac{e^{iq_0 r}}{4\pi r} \left(iq_0 - \frac{1}{r} \right) \exp(-iq_0 \hat{\mathbf{r}} \cdot \mathbf{r}'), \quad (20.65)$$

in (20.57) and (20.59), it is seen that the electric and magnetic fields, generated by a spin current density of the form given in (20.60), sufficiently far from the source region becomes

$$\mathbf{E}_T(\mathbf{r}; \omega) = \frac{i\mu_0\omega}{4\pi} \frac{e^{iq_0 r}}{r} \boldsymbol{\alpha}(q_0 \hat{\mathbf{r}}) \times \boldsymbol{\beta}(\omega), \quad (20.66)$$

and

$$\mathbf{B}(\mathbf{r}; \omega) = \frac{\mu_0}{4\pi} \frac{e^{iq_0 r}}{r} \left(iq_0 - \frac{1}{r} \right) \hat{\mathbf{r}} \times (\boldsymbol{\alpha}(q_0 \hat{\mathbf{r}}) \times \boldsymbol{\beta}(\omega)), \quad (20.67)$$

where

$$\boldsymbol{\alpha}(q_0 \hat{\mathbf{r}}) = \int_{-\infty}^{\infty} \boldsymbol{\alpha}(\mathbf{r}') \exp(-iq_0 \hat{\mathbf{r}} \cdot \mathbf{r}') d^3 r' \quad (20.68)$$

is the Fourier integral transform of the (frozen) spatial part of $\mathbf{J}^{\text{spin}}(\mathbf{r}', t)$. The vectorial Fourier variable $q_0 \hat{\mathbf{r}}$ has a direction given by the unit vector pointing from the origo of the coordinate system towards the point of observation for the field, and a magnitude proportional to the angular frequency of the field. Asymptotically, i.e., for $q_0 r \rightarrow \infty$, the mid-field term in $\mathbf{B}(\mathbf{r}; \omega)$ is negligible.

20.3.2 Emission from an Isotropic Microscopic Source

If the linear extension of the spin source is much smaller than all relevant electromagnetic wavelengths one may use the Taylor series expansion

$$\exp(-iq_0\hat{\mathbf{r}} \cdot \mathbf{r}') = 1 - iq_0\hat{\mathbf{r}} \cdot \mathbf{r}' + \dots \quad (20.69)$$

when calculating $\alpha(q_0\hat{\mathbf{r}})$. Hence,

$$\alpha(q_0\hat{\mathbf{r}}) = \int_{-\infty}^{\infty} \alpha(\mathbf{r}') d^3 r' - iq_0\hat{\mathbf{r}} \cdot \int_{-\infty}^{\infty} \mathbf{r}' \alpha(\mathbf{r}') d^3 r' + \dots \quad (20.70)$$

A further simplification is obtained if the frozen particle wave function is isotropic, i.e., $\psi(\mathbf{r}) = \psi(|\mathbf{r}|)$. For this case one has from (20.61)

$$\alpha(\mathbf{r}) = \frac{q\hbar}{2m} \hat{\mathbf{r}} \frac{\partial}{\partial r} |\psi(r)|^2. \quad (20.71)$$

Since $\alpha(\mathbf{r})$ now is an uneven function of x , y and z the first term on the right side of (20.70) vanishes. By retaining then only the leading term one has

$$\alpha(q_0\hat{\mathbf{r}}) = -iq_0\hat{\mathbf{r}} \cdot \mathbf{I}, \quad (20.72)$$

where

$$\mathbf{I} = \frac{q\hbar}{2m} \int_{-\infty}^{\infty} \frac{\mathbf{r}\mathbf{r}}{r} \frac{\partial}{\partial r} |\psi(r)|^2 d^3 r. \quad (20.73)$$

For symmetry reasons only the diagonal elements $(\mathbf{I})_{ii}$ [$i = (x, y, z)$] are non-vanishing, and the magnitudes of the three are equal of course. Altogether, one therefore obtains $\mathbf{I} = I\mathbf{U}$, where

$$I = \frac{q\hbar}{2m} \int_{-\infty}^{\infty} \frac{z^2}{r} \frac{\partial}{\partial r} |\psi(r)|^2 d^3 r. \quad (20.74)$$

Using spherical coordinates, the reader may easily verify that I is given by the one-dimensional integral

$$I = \frac{2\pi}{3} \frac{q\hbar}{m} \int_0^{\infty} r^3 \frac{\partial}{\partial r} |\psi(r)|^2 dr. \quad (20.75)$$

For an isotropic microscopic one-particle spin-1/2 source we thus have in lowest order

$$\alpha(q_0\hat{\mathbf{r}}) = -iq_0 I \hat{\mathbf{r}}. \quad (20.76)$$

In photon wave mechanics, the analytical fields $\mathbf{E}_T^{(+)}(\mathbf{r}; \omega)$ and $\mathbf{B}^{(+)}(\mathbf{r}; \omega)$ are needed. These follows from (20.66) and (20.67) with the replacement $\beta(\omega) \Rightarrow \beta^{(+)}(\omega)$. The magnitudes of the analytical fields are proportional to the magnitude of $\beta^{(+)}(\omega)$. For a one-photon spin source the relevant amplitude of $\beta^{(+)}(\omega)$ can be obtained by means of the procedure described in Sect. 18.3. From now on we assume that $\beta^{(+)}(\omega) = \langle \sigma \rangle^{(+)}(\omega)$ has been adjusted to its proper one-photon value. Leaving out the mid-field term from the magnetic field, the one-photon far fields are given by

$$\mathbf{e}_T^{(+)}(\mathbf{r}; \omega) = \frac{\mu_0 \omega^2 I}{4\pi c_0} \frac{e^{iq_0 r}}{r} \hat{\mathbf{r}} \times \boldsymbol{\beta}^{(+)}(\omega), \quad (20.77)$$

$$\mathbf{b}^{(+)}(\mathbf{r}; \omega) = \frac{\mu_0 \omega^2 I}{4\pi c_0^2} \frac{e^{iq_0 r}}{r} \hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \boldsymbol{\beta}^{(+)}(\omega)), \quad (20.78)$$

for an isotropic microscopic spin source. The photon (embryo) spinor related to (20.77) and (20.78) has the following form (cf. (16.23) and (18.61)) in the space–frequency domain:

$$\boldsymbol{\Psi}(\mathbf{r}; \omega) = \frac{\mu_0 \omega^2 I}{4\pi c_0} \sqrt{\frac{\epsilon_0}{2}} \frac{e^{iq_0 r}}{r} \left[\begin{pmatrix} 1 \\ 1 \end{pmatrix} \hat{\mathbf{r}} \times \boldsymbol{\beta}^{(+)}(\omega) + i \begin{pmatrix} 1 \\ -1 \end{pmatrix} \hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \boldsymbol{\beta}^{(+)}(\omega)) \right]. \quad (20.79)$$

Since the Fourier transform of the function $-\omega^2 \boldsymbol{\beta}^{(+)}(\omega)$ is $\ddot{\boldsymbol{\beta}}^{(+)}(t)$ use of the folding theorem immediately leads to the following expression for the wave function (embryo) in the space–time domain:

$$\begin{aligned} \boldsymbol{\Psi}(\mathbf{r}, t) = & -\frac{\mu_0 I}{4\pi c_0} \sqrt{\frac{\epsilon_0}{2}} \frac{1}{r} \int_{-\infty}^{\infty} \delta\left(\frac{r}{c_0} - t + t'\right) \\ & \times \left[\begin{pmatrix} 1 \\ 1 \end{pmatrix} \hat{\mathbf{r}} \times \ddot{\boldsymbol{\beta}}^{(+)}(t') + i \begin{pmatrix} 1 \\ -1 \end{pmatrix} \hat{\mathbf{r}} \times (\hat{\mathbf{r}} \times \ddot{\boldsymbol{\beta}}^{(+)}(t')) \right] dt', \end{aligned} \quad (20.80)$$

or equivalently in retarded-time notation

$$\begin{aligned} \boldsymbol{\Psi}(\mathbf{r}, t) = & -\frac{\mu_0 I}{4\pi c_0} \sqrt{\frac{\epsilon_0}{2}} \frac{1}{r} \left[\begin{pmatrix} 1 \\ 1 \end{pmatrix} \hat{\mathbf{r}} \times \frac{d^2}{dt^2} \langle \boldsymbol{\sigma} \rangle^{(+)}([t]) \right. \\ & \left. + i \begin{pmatrix} 1 \\ -1 \end{pmatrix} \hat{\mathbf{r}} \times \left(\hat{\mathbf{r}} \times \frac{d^2}{dt^2} \langle \boldsymbol{\sigma} \rangle^{(+)}([t]) \right) \right]. \end{aligned} \quad (20.81)$$

In a hydrogen atom, the magnetic interaction between the proton and electron spins gives rise to a so-called hyperfine structure of the electron levels. The ground state (1s) has no fine structure, and since the electron in this state has no orbital angular momentum, the hyperfine split 1s state is a paradigm of a pure spin-1/2 source. The far-field wave function of a radio-frequency photon emitted from the isotropic 1s state can be calculated from (20.81) once the time dependence of the quantum mechanical mean value $\langle \boldsymbol{\sigma} \rangle(t)$ is known, and the approximate value for the integral in (20.75) has been obtained. In the hydrogen ground state the orbital part of the electron wave function is given by $\psi(r) = (\pi a_0^3)^{-1/2} \exp(-r/a_0)$, where a_0 is the Bohr radius, and an elementary calculation results in

$$I = \frac{e\hbar}{2m}, \quad (20.82)$$

where e is the numerical value of the electron charge. In [180], the photon emission process from the hyperfine ground-state dynamics is studied in the case where a uniform static magnetic field splits the two levels into four (Zeeman effect).

Chapter 21

One-Particle Position Operators and Spatial Localization

21.1 Nonrelativistic Particle

In the so-called standard model of particle physics one attempts to describe all physical phenomena in terms of the properties and interactions of a (small) number of different particles which are assumed to be elementary in the sense that they are treated as point particles without internal structure (excited states). The leptons (electron, muon, tauon, and the associated three neutrino's), quarks (six types) and their antiparticles all are spin-1/2 fermions. The carriers of the interactions between these spin-1/2 particles, the gauge bosons ($W^\pm$ and Z^0 bosons, gluons, and the photons), are spin-1 bosons. Among these elementary point-particles the electron and the photon are the ones of relevance in quantum electrodynamics.

Let us now ask the following question: To what extent can a point-particle be localized in space? If a particle's position is to be measured in quantum mechanics, the various positions in space, $\mathbf{r}_0$, should be the eigenvalues of some position operator (observable) $\hat{\mathbf{r}}$. The eigenvalue equation for $\hat{\mathbf{r}}$ was written down in (11.58), and the requirements that the position eigenvectors satisfy (1) the generalized orthonormality condition and (2) the completeness theorem were expressed in (11.59) and (11.60), respectively. In nonrelativistic quantum mechanics, the scalar product of two wave functions is given by

$$\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^*(\mathbf{r}) \phi(\mathbf{r}) d^3r. \quad (21.1)$$

in the configuration-space representation, cf. (11.64). By combining (11.65) and (11.67) it appears that the nonrelativistic particle position operator is just $\hat{\mathbf{r}} = \mathbf{r}$ in the $\{|\mathbf{r}\rangle\}$ representation, a well known textbook result. By means of the complex conjugate of the Fourier integral $[\psi(\mathbf{p}/\hbar) \equiv \psi(\mathbf{p})]$

$$\psi(\mathbf{r}) = (2\pi\hbar)^{-3} \int_{-\infty}^{\infty} \psi(\mathbf{p}) \exp\left(\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}\right) d^3p, \quad (21.2)$$

and a similar integral for $\phi(\mathbf{r})$, the scalar product in (21.1) takes the form

$$\langle \psi | \phi \rangle = (2\pi\hbar)^{-3} \int_{-\infty}^{\infty} \psi^*(\mathbf{p}) \phi(\mathbf{p}) d^3 p \quad (21.3)$$

in the momentum representation, cf. the Parseval–Plancherel relation (9.56). From the inverse transformation to the one in (21.2) it may easily be shown that $\mathbf{r}\psi(\mathbf{r})$ has a Fourier transform $i\hbar\nabla_{\mathbf{p}}\psi(\mathbf{p})$. Thus, $\hat{\mathbf{r}} = i\hbar\nabla_{\mathbf{p}}$ is the $\{|\mathbf{p}\rangle\}$ representation of the nonrelativistic position operator. Elementary calculations show that the position operator is Hermitian with respect to the nonrelativistic scalar product.

21.2 Massive Relativistic Particle of Zero Spin

21.2.1 Position Operator

It is obvious that a factor $(2\pi\hbar)^{-3/2}$ can be absorbed in the $\mathbf{p}$ -space wave function without changing the physics. This gives us the nonrelativistic scalar product form:

$$\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^*(\mathbf{p}) \phi(\mathbf{p}) d^3 p. \quad (21.4)$$

The discussion in Sect. 16.1.4 makes it clear that the relativistic Lorentz-invariant scalar product for a massive spinless particle (Klein–Gordon particle) can be written as

$$\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^*(\mathbf{p}) \phi(\mathbf{p}) \frac{d^3 p}{[p^2 + (mc_0)^2]^{1/2}} \quad (21.5)$$

in the momentum representation, leaving out a possible but unessential prefactor to the integral. The form of the scalar product implies that the wave function in momentum space has the dimension $(MOMENTUM)^{1/2}$ since the free-particle wave function is normalized in the Dirac sense (11.59). We shall by a direct calculation verify this statement soon. The scalar product in (21.5) is meaningful only when applied to positive energy wave functions, and it satisfies all the properties required of a scalar product in quantum mechanics, among others the relation in (11.7).

The position operator in the nonrelativistic (NR) theory I now rename $\hat{\mathbf{r}}_{\text{NR}}$. Thus,

$$\hat{\mathbf{r}}_{\text{NR}} = i\hbar\nabla_{\mathbf{q}} \quad (21.6)$$

in the momentum representation. In the relativistic theory, the naive position operator $\hat{\mathbf{r}}_{\text{NR}}$ is no longer Hermitian. To prove this, we start from the scalar product in (21.5) and form the relativistic mean value of $\hat{\mathbf{r}}_{\text{NR}}$, i.e.,

$$\langle \psi | \hat{\mathbf{r}}_{\text{NR}} | \phi \rangle = i\hbar \int_{-\infty}^{\infty} \psi^*(\mathbf{p}) (\nabla_{\mathbf{p}} \phi(\mathbf{p})) \frac{d^3 p}{[p^2 + (mc_0)^2]^{1/2}}. \quad (21.7)$$

Since

$$\nabla_p \left\{ \frac{\psi^*(p)}{[p^2 + (mc_0)^2]^{1/2}} \right\} = \frac{\nabla_p \psi^*(p)}{[p^2 + (mc_0)^2]^{1/2}} - \frac{p \psi^*(p)}{[p^2 + (mc_0)^2]^{3/2}}, \quad (21.8)$$

a partial integration of (21.7) gives

$$\begin{aligned} \langle \psi | \hat{r}_{NR} | \phi \rangle &= \int_{-\infty}^{\infty} \left[i \hbar \left(\nabla_p - \frac{p}{p^2 + (mc_0)^2} \right) \psi(p) \right]^* \phi(p) \frac{d^3 p}{[p^2 + (mc_0)^2]^{3/2}}, \end{aligned} \quad (21.9)$$

because the surface terms at infinity vanish. It appears from (21.9) that

$$\begin{aligned} \langle \psi | \hat{r}_{NR} | \phi \rangle &= \langle \hat{r}_{NR} \psi | \phi \rangle \\ &+ i \hbar \int_{-\infty}^{\infty} \psi^*(p) \phi(p) \frac{p d^3 p}{[p^2 + (mc_0)^2]^{3/2}}, \end{aligned} \quad (21.10)$$

and this result proves that $\hat{r}_{NR}$ is not Hermitian. It is obvious from (21.10) how a Hermitian operator closely related to $\hat{r}_{NR}$ can be constructed, however. Hence, if one transfers half of the last term in (21.10) from the right to the left side of the equation it follows that

$$\langle \psi | \hat{r} | \phi \rangle = \langle \hat{r} \psi | \phi \rangle, \quad (21.11)$$

where

$$\hat{r} = i \hbar \left\{ \nabla_p - \frac{p}{2[p^2 + (mc_0)^2]} \right\}. \quad (21.12)$$

Within the framework of the relativistic scalar product (21.5), where the Lorentz-invariant volume element is $d^3 p / [p^2 + (mc_0)^2]^{1/2}$, the operator $\hat{r}$ in (21.12) is Hermitian. The new operator satisfies the dyadic commutator relation

$$\begin{aligned} [\hat{r}, \hat{p}] &= \left[i \hbar \left\{ \nabla_p - \frac{p}{2[p^2 + (mc_0)^2]} \right\}, p \right] \\ &= [\hat{r}_{NR}, \hat{p}] = i \hbar \hat{1}, \end{aligned} \quad (21.13)$$

where $\hat{1}$ is the unit matrix operator. The Hermitian $\hat{r}$ operator therefore is the canonical conjugate operator of the momentum operator, and thus an acceptable relativistic one-particle position operator for a massive spinless particle.

21.2.2 Eigenstates of the Position Operator: Localization in Configuration Space

Let us now determine the eigenfunctions for the relativistic position operator, starting in the momentum representation, where the eigenvalue equation may be written

$$\hat{\mathbf{r}}(\mathbf{p})\psi_{r_0}(\mathbf{p}) = \mathbf{r}_0\psi_{r_0}(\mathbf{p}). \quad (21.14)$$

An eigenstate of the position operator $\hat{\mathbf{r}}$ (21.12), which corresponds to a “localization” at $\mathbf{r}_0$, is denoted by $\psi_{r_0}(\mathbf{p})$. The precise meaning of the word *localization* will soon become clear. To solve the eigenvalue problem we insert the ansatz

$$\psi_{r_0}(\mathbf{p}) = \psi_0(\mathbf{p})\exp\left(-\frac{i}{\hbar}\mathbf{r}_0 \cdot \mathbf{p}\right) \quad (21.15)$$

into (21.14). As the reader may convince himself of, this leads to the following differential equation for $\psi_0(\mathbf{p})$:

$$\nabla_{\mathbf{p}}\psi_0(\mathbf{p}) = \frac{\mathbf{p}}{2[p^2 + (mc_0)^2]}\psi_0(\mathbf{p}). \quad (21.16)$$

Since the gradient of $\psi_0(\mathbf{p})$ is in the direction of the $\mathbf{p}$ -vector, ψ_0 can only be a function of the numerical magnitude of the momentum that is $\psi_0(\mathbf{p}) = \psi_0(p)$. The equation for $\psi_0(p)$ becomes

$$\frac{d\psi_0(p)}{dp} = \frac{p\psi_0(p)}{2[p^2 + (mc_0)^2]}, \quad (21.17)$$

or equivalently

$$4\frac{d\psi_0(p)}{\psi_0(p)} = \frac{dp^2}{p^2 + (mc_0)^2}. \quad (21.18)$$

By integration of the separated equation one immediately obtains

$$\psi_0(p) = [p^2 + (mc_0)^2]^{1/4}. \quad (21.19)$$

The eigenfunction for the relativistic position operator belonging to the vectorial eigenvalue $\mathbf{r}_0$ thus is given by

$$\psi_{r_0}(\mathbf{p}) = [p^2 + (mc_0)^2]^{1/4} \exp\left(-\frac{i}{\hbar}\mathbf{r}_0 \cdot \mathbf{p}\right), \quad (21.20)$$

apart from an arbitrary multiplicative factor. This factor cannot be determined by normalization, because the wave function of our free particle is unnormalizable, as one might have anticipated. As mentioned earlier, the dimension of the relativistic wave function in momentum space is $(\text{MOMENTUM})^{1/2}$ (with the scalar product defined by (21.5)). In the nonrelativistic limit, $p/(mc_0) \rightarrow 0$, the wave function becomes a plane wave, $\exp(-i\mathbf{r}_0 \cdot \mathbf{p}/\hbar)$. This is the expected result, as we shall see soon.

The wave function $\psi_{r_0}(\mathbf{p})$ can be transformed back to configuration space by means of (21.2). Thus,

$$\psi_{r_0}(\mathbf{r}) = (2\pi\hbar)^{-3} \int_{-\infty}^{\infty} [p^2 + (mc_0)^2]^{1/4} \exp\left[\frac{i}{\hbar}(\mathbf{r} - \mathbf{r}_0) \cdot \mathbf{p}\right] d^3p \quad (21.21)$$

within an arbitrary constant. Let us first consider the nonrelativistic limit of (21.21). For $p/(mc_0) \rightarrow 0$, the factor to the exponential function approaches a constant $(mc_0)^{1/2}$, which one with no loss of generality can absorb in the undetermined amplitude of the nonrelativistic (NR) wave function of the free particle, $\psi_{r_0}^{\text{NR}}$. Hence, from

$$\psi_{r_0}^{\text{NR}}(\mathbf{r}) = (2\pi\hbar)^{-3} \int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}(\mathbf{r} - \mathbf{r}_0) \cdot \mathbf{p}\right] d^3p = \delta(\mathbf{r} - \mathbf{r}_0), \quad (21.22)$$

it is seen that $\psi_{r_0}^{\text{NR}}(\mathbf{r})$ is the generalized wave function of a particle completely localized in space at $\mathbf{r} = \mathbf{r}_0$. In the framework of nonrelativistic quantum mechanics, it is thus possible to achieve a perfect localization of a point particle. The set of delta functions labeled by the continuous vectorial index $\mathbf{r}_0$ form a generalized basis because they satisfy the Dirac orthonormalization

$$\langle \psi_{r'_0}^{\text{NR}}(\mathbf{r}) | \psi_{r_0}^{\text{NR}}(\mathbf{r}) \rangle = \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}_0) d^3r = \delta(\mathbf{r}_0 - \mathbf{r}'_0) \quad (21.23)$$

and completeness

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi_{r_0}^{\text{NR}}(\mathbf{r})\rangle \langle \psi_{r'_0}^{\text{NR}}(\mathbf{r}')| d^3r_0 &= \int_{-\infty}^{\infty} \delta(\mathbf{r} - \mathbf{r}_0) \delta(\mathbf{r}' - \mathbf{r}_0) d^3r_0 \\ &= \delta(\mathbf{r} - \mathbf{r}') \end{aligned} \quad (21.24)$$

relations.

In the ultrarelativistic limit ($p/(mc_0) \rightarrow \infty$), as well as in the massless limit ($m \rightarrow 0$), the wave function in (21.21) is given by the integral

$$\psi_{r_0}(\mathbf{r}) = \frac{\hbar^{1/2}}{(2\pi)^3} \int_{-\infty}^{\infty} q^{1/2} \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}_0)] d^3q, \quad (21.25)$$

as one immediately finds using the substitution $\mathbf{p} = \hbar\mathbf{q}$. The integral can be evaluated by the same procedure as used in Sect. 15.5, and the regularized wave function hence becomes

$$\psi_{r_0}(\mathbf{r}) = -\frac{3}{(4\pi)^2} \hbar^{1/2} |\mathbf{r} - \mathbf{r}_0|^{-7/2}. \quad (21.26)$$

In configuration ($\mathbf{r}$) space, the relativistic eigenstate corresponding to a localization at $\mathbf{r}_0$ is not a delta function. In the ultrarelativistic and massless limits, the localization of the wave function exhibits a power-law dependence of the type $|\mathbf{r} - \mathbf{r}_0|^{-7/2}$. In the framework of the complex field theory of the photon, we have realized in Sect. 15.5 that the electromagnetic field corresponding to an *assumed*

analytic completely localized wave function also would spread out around the point $\mathbf{r}_0$ according to $|\mathbf{r} - \mathbf{r}_0|^{-7/2}$.

We now turn our attention towards the general case, given by (21.21). In order to give a somewhat more precise meaning of what is meant by the words “a localized state,” let us calculate the scalar product of the two eigenfunctions of the position operator with different eigenvalues, say $\mathbf{r}_0$ and $\mathbf{r}'_0$, i.e.,

$$\langle \psi_{\mathbf{r}'_0} | \psi_{\mathbf{r}_0} \rangle = \int_{-\infty}^{\infty} \psi_{\mathbf{r}'_0}^*(\mathbf{p}) \psi_{\mathbf{r}_0}(\mathbf{p}) \frac{d^3 p}{[p^2 + (mc_0)^2]^{1/2}}, \quad (21.27)$$

cf. (21.5). By means of (21.20) we immediately obtain

$$\langle \psi_{\mathbf{r}'_0} | \psi_{\mathbf{r}_0} \rangle = \int_{-\infty}^{\infty} \exp \left[\frac{i}{\hbar} (\mathbf{r}'_0 - \mathbf{r}_0) \cdot \mathbf{p} \right] d^3 p = (2\pi\hbar)^3 \delta(\mathbf{r}_0 - \mathbf{r}'_0). \quad (21.28)$$

The two states thus are orthogonal for $\mathbf{r}_0 \neq \mathbf{r}'_0$. For relativistic dynamics it is altogether reasonable to require localized states to satisfy: (1) That the set of all localized states are invariant under rotations and spatial inversion about the point of localization and (2) that a state localized at $\mathbf{r}_0$ after any non-zero spatial displacement becomes orthogonal to the manifold of states localized at $\mathbf{r}_0$ [248, 291]. The position eigenfunctions in configuration space are given by (21.21). In polar coordinates, with the polar axis along the $\mathbf{r} - \mathbf{r}_0$ direction, the angular integrations are easy to carry out. Doing this, one obtains

$$\psi_{\mathbf{r}_0}(\mathbf{r}) = \frac{2(2\pi\hbar)^{-2}}{|\mathbf{r} - \mathbf{r}_0|} \int_0^{\infty} p [p^2 + (mc_0)^2]^{1/4} \sin \left(|\mathbf{r} - \mathbf{r}_0| \frac{p}{\hbar} \right) dp, \quad (21.29)$$

and thereafter with the substitution $p = mc_0 x$

$$\psi_{\mathbf{r}_0}(\mathbf{r}) = 2(2\pi\hbar)^{-2} \frac{(mc_0)^{3/2}}{|\mathbf{r} - \mathbf{r}_0|} F \left(\frac{mc_0}{\hbar} |\mathbf{r} - \mathbf{r}_0| \right), \quad (21.30)$$

where

$$F \left(\frac{mc_0}{\hbar} |\mathbf{r} - \mathbf{r}_0| \right) = \int_0^{\infty} x (1 + x^2)^{1/4} \sin \left(\frac{mc_0}{\hbar} |\mathbf{r} - \mathbf{r}_0| x \right) dx. \quad (21.31)$$

It appears that the function F only depends on the ratio $|\mathbf{r} - \mathbf{r}_0|/\lambda_C$, where

$$\lambda_C = \frac{\hbar}{mc_0} \quad (21.32)$$

is the particle's Compton wavelength divided by 2π . It may be shown that $F(z) \approx z^{-5/4} \exp(-z)$ for $z \gg 1$ [291]. This means that the wave function in configuration space, $\psi_{\mathbf{r}_0}(\mathbf{r})$, is smeared out over a region of linear extension as the Compton

wavelength around the point of localization, $\mathbf{r}_0$. On a length scale qualitatively smaller than λ_C relativistic quantum mechanics must be replaced by quantum field theory [157].

21.3 Massless Spin-One Particle (Photon)

21.3.1 Transverse Eigenstates in Momentum Space

One might be tempted to believe that a photon position operator could be obtained from (21.12) setting $m = 0$. This cannot be so, because the consideration in Sect. 21.2 apply to spinless particles. Depending on the definition one chooses for the wave function of the free photon, the eigenvectors must be vectors with three (four-potential theory) or six (complex field theory, energy wave function formalism) components, and a position operator therefore a 3×3 or 6×6 matrix. To keep the analysis as simple as possible let us assume that we base our description on the potentials. A first guess for a photon position operator in momentum space might be

$$\hat{\mathbf{r}}_{ij} = i\hbar \left(\nabla_p - \frac{\mathbf{p}}{2p^2} \right) \delta_{ij}, \quad (21.33)$$

where $i, j = 1, 2, 3$. Each component of $\hat{\mathbf{r}}_{ij}$ is a vector, and the position operator in (21.33) only has nonvanishing diagonal elements. Bearing in mind that the photon wave function $\mathbf{A}_T^{(+)}(\mathbf{p}; t)$ is transversely polarized, i.e., $\mathbf{p} \cdot \mathbf{A}_T^{(+)}(\mathbf{p}; t) = 0$, a serious problem arises for the suggestion in (21.33). Thus, when the gradient operator acts on $\mathbf{A}_T^{(+)}$ the resulting three-vector necessarily obtains a longitudinal component, and $\hat{\mathbf{r}}_{ij}$ alone for this reason cannot serve as a photon position operator. How do we get around this problem? In Sect. 21.2, we started from the position operator in (21.12), and we then determined its eigenvectors (21.20). A possible way out of our problem is to follow the opposite procedure: (1) Start from an eigenvector with the desired properties, (2) let the ∇_p -operator act on this state, and (3) subtract the longitudinal effect produced by the gradient operator.

With the result in (21.20) in mind, let us consider the three three-vector momentum space wave functions (time dependence omitted from the notation for brevity)

$$\psi_{\mathbf{r}_0, s}(\mathbf{p}) = A_s p^{1/2} \hat{\mathbf{e}}_{ps} \exp \left(-\frac{i}{\hbar} \mathbf{r}_0 \cdot \mathbf{p} \right), \quad s = 1, 2, 3, \quad (21.34)$$

where, with respect to $\mathbf{p}$, $\hat{\mathbf{e}}_{p1}$ and $\hat{\mathbf{e}}_{p2}$ are transverse unit vectors, and $\hat{\mathbf{e}}_{p3}$ is a longitudinal unit vector. The quantity A_s is a constant (depending in general on s). Although only the two transverse wave functions ($s = 1, 2$) are needed, the longitudinal wave function ($s = 3$) is kept for generality. The presence of the $p^{1/2}$ -factor in (21.34) ensures that the scalar product for the two arbitrary three-vector wave functions $\psi(\mathbf{p})$ and $\phi(\mathbf{p})$ has the relativistic form for massless particles, i.e.,

$$\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^\dagger(\mathbf{p}) \phi(\mathbf{p}) \frac{d^3 p}{p}, \quad (21.35)$$

cf. (21.5). Since

$$\langle \psi_{\mathbf{r}'_0, s'} | \psi_{\mathbf{r}_0, s} \rangle = |A_s|^2 \delta(\mathbf{r}_0 - \mathbf{r}'_0) \delta_{ss'} \quad (21.36)$$

the states in (21.34) are orthonormalized in the Dirac sense.

21.3.2 Dyadic Photon Position Operator

Following the procedure indicated in the text above (21.34) we let the x -component of the operator $i\hbar \nabla_p$ act on each of the wave functions in (21.34). This gives

$$\begin{aligned} i\hbar(\nabla_p)_x \psi_{\mathbf{r}_0, s}(\mathbf{p}) \\ = i\hbar \left(\frac{p_x}{2p^2} - \frac{i x_0}{\hbar} \right) \psi_{\mathbf{r}_0, s}(\mathbf{p}) + i\hbar A_s p^{1/2} \left(\frac{\partial}{\partial p_x} \hat{\mathbf{e}}_{ps} \right) \exp \left(-\frac{i}{\hbar} \mathbf{r}_0 \cdot \mathbf{p} \right). \end{aligned} \quad (21.37)$$

To bring (21.37) into a form where it appears as an eigenvalue equation, the last term must be rewritten so that the wave function $\psi_{\mathbf{r}_0, s}(\mathbf{p})$ enters explicitly. Such a goal is readily achieved since

$$\frac{\partial}{\partial p_x} \hat{\mathbf{e}}_{ps} = \left[\sum_{s'=1}^3 \left(\frac{\partial}{\partial p_x} \hat{\mathbf{e}}_{ps'} \right) \hat{\mathbf{e}}_{ps'} \right] \cdot \hat{\mathbf{e}}_{ps}, \quad (21.38)$$

due to the fact that the polarization unit vectors are orthogonal. By combining (21.37) and (21.38), and rearranging terms, one obtains

$$i\hbar \left\{ \left[(\nabla_p)_x - \frac{p_x}{2p^2} \right] U - \sum_{s'=1}^3 \left(\frac{\partial}{\partial p_x} \hat{\mathbf{e}}_{ps'} \right) \hat{\mathbf{e}}_{ps'} \right\} \cdot \psi_{\mathbf{r}_0, s}(\mathbf{p}) = x_0 \psi_{\mathbf{r}_0, s}(\mathbf{p}). \quad (21.39)$$

The result in (21.39) suggests that the quantity

$$\hat{\mathbf{r}}_{ij} = i\hbar \left\{ \delta_{ij} \left(\nabla_p - \frac{\mathbf{p}}{2p^2} \right) - \sum_{s=1}^3 [\nabla_p (\hat{\mathbf{e}}_{ps})_i] (\hat{\mathbf{e}}_{ps})_j \right\} \quad (21.40)$$

may serve as the ij th element of a photon position operator, with the related eigenvalue equation

$$\sum_{j=1}^3 \hat{\mathbf{r}}_{ij} (\psi_{\mathbf{r}_0, s})_j = \mathbf{r}_0 (\psi_{\mathbf{r}_0, s})_i. \quad (21.41)$$

For free photons only the eigenvectors for $s = 1$ and 2 are of relevance.

21.3.3 The Photon Position Operator Problem in Configuration Space

At this point it might be tempting to seek to transform the $\mathbf{p}$ -space wave functions in (21.34) back to $\mathbf{r}$ -space with the help of the Fourier integral transformation in (21.2). Omitting the arbitrary multiplicative factor A_s , the position operator eigenfunction for mode s formally is given by the integral expression

$$\psi_{r_0,s}(\mathbf{r}) = (2\pi\hbar)^{-3} \int_{-\infty}^{\infty} p^{1/2} \hat{\mathbf{e}}_{ps}(\hat{\mathbf{p}}) \exp \left[\frac{i}{\hbar} (\mathbf{r} - \mathbf{r}_0) \cdot \mathbf{p} \right] d^3 p. \quad (21.42)$$

It is not unexpected that (21.42) tells us that the wave function $\psi_{r_0,s}(\mathbf{r})$ is (1) smeared out in configuration space around the point of localization and (2) singular at $\mathbf{r} = \mathbf{r}_0$. The result in (21.42) is problematic, however, because the integral is not convergent, and if one tries to use the regularization procedure described in Sect. 15.7 the transverse ($s = 1, 2$) and longitudinal ($s = 3$) character of the wave functions are lost. In order to pinpoint the cause for this, let us take a closer look at the problem. For a given longitudinal unit vector

$$\hat{\mathbf{e}}_{p3} = p^{-1}(p_x, p_y, p_z) \quad (21.43)$$

we make the choice

$$\hat{\mathbf{e}}_{p1} = p^{-2}(-p_x p_z, -p_y p_z, p_x^2 + p_y^2), \quad (21.44)$$

$$\hat{\mathbf{e}}_{p2} = p^{-1}(p_y, -p_x, 0), \quad (21.45)$$

for the transverse unit vectors, and assume that the z -axis of our Cartesian coordinate system is placed along the $\mathbf{r} - \mathbf{r}_0$ -direction. In polar coordinates with the polar axis along the $\mathbf{r} - \mathbf{r}_0$ -direction, the integrations over the azimuth and polar angles are easy to carry out. For the $s = 1$ mode, one thus obtains

$$\psi_{r_0,1}(\mathbf{r}) = 8\pi\hbar^{-3} \frac{\mathbf{r} - \mathbf{r}_0}{|\mathbf{r} - \mathbf{r}_0|^{9/2}} \int_0^\infty (x^{-1/2} \sin x - x^{1/2} \cos x) dx. \quad (21.46)$$

Although the remaining integral can be done using the regularization procedure in Sect. 15.7 it is not necessary to do so, since the reader readily verify that $\nabla \cdot \psi_{r_0,1}(\mathbf{r}) \neq 0$. The result obtained for $\psi_{r_0,1}(\mathbf{r})$ is, therefore, not divergence-free as one must require. For $s = 2$, the angular integration over the azimuth angle leads immediately to the unacceptable result $\psi_{r_0,2}(\mathbf{r}) = 0$.

Part III
Quantum Electrodynamic Theory

Chapter 22

Near Fields and QED

22.1 The Zoo of Photons

In the famous *Drei-Männer-Arbeit* from 1926, one of the central papers on matrix mechanics, Born, Heisenberg, and Jordan quantized the free radiation field [292]. For simplicity, they worked in one space dimension and ignored the polarization of the electromagnetic waves. As anticipated by Ehrenfest twenty years earlier [293], the field behaves like a sum of independent harmonic oscillators. Upon quantization, the photon and (infinite) zero-point energy concepts entered the stage. The *Drei-Männer-Arbeit*, together with Dirac's studies of the spontaneous emission process [294, 295], mark the birth of quantum electrodynamics (QED), and in a broader sense quantum field theory [296–299]. In modern field theory, photons, electrons, together with all other fundamental “particles” are elementary quantum excitations of some sort of underlying field [156, 157].

The photons are quantities belonging to the free electromagnetic field [53, 74, 117, 156, 178, 236, 237, 243, 300–305], and the superposition principle of quantum mechanics allows one-photon states to appear in a variety of different space-time forms. In order to observe the quantized structure of the radiation field, its interaction with matter (charged particles) *must* be analyzed. In the field–matter interaction processes photons are created and/or destroyed, so in a sense one may say that photons only come to “existence” during their birth and/or death process in space-time. The birth (death) process is a quantum statistical event, and the process only is brought to an end when the quantum statistics tells us that the photon with certainty has been created (destroyed).

In the nonrelativistic domain the Coulomb gauge most often is used in the description of quantum electrodynamic phenomena [178]. In this gauge only the transverse part of the electromagnetic field is quantized, and the related elementary quantum excitations are so-called transverse (T) photons. In quantum optics (and in most textbooks), the T -photons are those associated with a plane-wave quantization of the free electromagnetic field [74, 117, 178, 301–305]. In Sect. 23.1, we briefly review the standard quantization scheme leading to the introduction of the monochromatic plane-wave transverse photons. We also derive expressions for the Hamilton, momentum and spin operators of the transverse field.

Equivalent formulations of QED derived from the Coulomb gauge by a gauge transformation [178] are of interest in near-field QED, not least because such transformations allow one to see the field–matter interaction in the rim zone from other perspectives. Among the various gauges the Poincaré gauge [306–308] appears to be of special interest in near-field physics, and in Chap. 25 we study the quantum description in this gauge. The gauge function which brings one from the Coulomb gauge to the Poincaré gauge relates to a specific choice for the generalized polarization and magnetization, concepts we have discussed in some detail in the context of linear nonlocal response theory (Sects. 10.4 and 10.5). Since the conjugate field variables in the Poincaré gauge are the transverse part of the vector potential and the electric displacement field (multiplied by -1), the photons of the Poincaré gauge are of the transverse type.

In the relativistic domain, where the Lorentz invariance of the theoretical descriptions is of great importance, it is often preferably in the potential formulation of electrodynamics to use a gauge in which the Maxwell–Lorentz equations take a manifestly covariant form [130, 155, 309–313]. In a covariant gauge, also named a Lorenz gauge [147–152], the four-potential $\{A^\mu\}$ satisfies the Lorenz condition [150–152]

$$\partial_\mu A^\mu = 0, \quad (22.1)$$

cf. (2.13). In the covariant formulation of QED two new types of monochromatic plane-wave photons appear, viz., the scalar (S) photon and the longitudinal (L) photon, as we shall see in Chap. 29. Since only transverse electromagnetic fields can exist in free space the net effect of the quantized longitudinal and scalar fields must be zero. This is achieved by requiring that the physical field states in vacuum, $|\psi\rangle$, satisfy the subsidiary Gupta–Bleuler–Lorenz condition [155, 178, 314, 315]

$$\partial_\mu \hat{A}^{\mu(+)} |\psi\rangle = 0 \quad (22.2)$$

in all space–time points.

It has been pointed out by the present author that the Lorentz-covariant formulation of QED might be of interest also for *nonrelativistic* near-field physics [177, 180, 231], because the longitudinal part of the electromagnetic field plays an important role in the rim zone of matter. In a quantum setting the longitudinal electric field contains contribution from both the longitudinal and scalar photon fields. The role of the rim zone in near-field QED may be emphasized by replacing the L - and S -photons by two new photon types: The near-field (NF) and gauge (G) photons [177]. The NF- and G-photon fields both contain all information on the (quantized) longitudinal electric field, and therefore, only one of them needs to be used in near-field QED. In free space, no physical state can contain near-field photons. Mathematically, this is expressed by the subsidiary condition

$$\hat{a}_{\text{NF}}(\mathbf{q}) |\psi\rangle = 0, \quad \forall \mathbf{q}, \quad (22.3)$$

$\hat{a}_{\text{NF}}(\mathbf{q})$ being the annihilation operator for near-field photons belonging to mode $\mathbf{q}$. Gauge photons can “exist” in free space, but, they play no physical role. This statement is manifestly correct since a given nonvanishing gauge potential, A_G^μ , can be eliminated by a suitable gauge transformation within the Lorenz gauge.

22.1.1 One-Photon Wave Packets

Monochromatic plane-wave one-photon states can be superimposed (linearly) to give new single-photon states, e.g., of the wave packet type, as we shall learn in Chap. 26. A one-photon wave packet state is an eigenstate for the global photon number operator, but such a state is in general *not* an eigenstate of the global Hamilton operator, nor the global momentum operator, of the quantized transverse field. In general, a single-photon wave packet state therefore is not a stationary photon state. After all, the quantum mechanical mean value and (Heisenberg) uncertainty of the global Hamilton and momentum operators are time independent in free space. The relation to photon wave mechanics in the Riemann–Silberstein formulation comes via the introduction of so-called free photon-field operators [180, 213] for the two helicity states, and their mean values in a one-photon state equal the local one-photon energy density for the two helicity states [to the extent that a photon can be localized in space-time].

22.2 Near-Field Commutators

The question of the measurability of electromagnetic field quantities was investigated carefully by Bohr and Rosenfeld in 1933 [316], and further in 1950 [317]. Using a number of ingenious thought experiments involving test bodies, they showed that the commutators of fields express limitations in our ability to measure fields at space–time points separated by time-like intervals. In near-field electrodynamics not only commutators among the field operators $\hat{\mathbf{E}}_T$ and $\hat{\mathbf{B}}$ are of interest, but also commutators involving the transverse vector potential operator, $\hat{\mathbf{A}}_T$, must be studied. In particular the $[\hat{\mathbf{A}}_T, \hat{\mathbf{E}}_T]$ -commutator’s near-field part turns out to be of crucial importance for our understanding of, e.g., the spatial localization problem for photons and the quantum electrodynamic interaction between objects in rim-zone contact.

We begin our investigation in Sect. 24.2 with a calculation of free-field commutators for fields taken at different space-time points. In a sense one may claim that the *entanglement* phenomenon verified in a number of experimental studies, represents the most profound observable aspect of the Copenhagen interpretation of quantum theory [13, 267]. The peculiar *spatial nonlocality*, which is the basis of entanglement, here manifests itself in the near-field part of the commutator between the gauge invariant $\hat{\mathbf{A}}_T$ -operator and the $\hat{\mathbf{E}}_T$ -operator. In free space, where

this commutator exhibits translational invariance in space and time, one finds the following near-field (NF) result:

$$R^{-2} \mathbf{R} \cdot \left[\hat{\mathbf{A}}_{\text{T}}(\mathbf{R}, \tau), \hat{\mathbf{E}}_{\text{T}}(\mathbf{0}, 0) \right]_{\text{NF}} \cdot \mathbf{R} = \frac{\hbar}{i} \frac{\theta(R - c_0|\tau|)}{2\pi\epsilon_0 R^3}. \quad (22.4)$$

The Heaviside step function $\theta(R - c_0|\tau|)$ indicates the presence of correlation of space-like ($R > c_0|\tau|$) events. In a wide perspective the result rules out the possibility for a deterministic description of photon trajectories via local hidden variables [13, 264, 265, 267]. Whether or not there *are* photon trajectories beyond the geometrical optical domain no one knows [265]. The foundation of our present quantum electrodynamical theory, including the detection process (measurement problem) for photons, makes it difficult for me to believe in the notion that a localized light quantum can propagate along a definite trajectory (a nonlocal pilot-wave theory for photons [264–267]).

In the presence of field–matter interaction the result for the $[\hat{\mathbf{A}}_{\text{T}}, \hat{\mathbf{E}}_{\text{T}}]$ -commutator becomes more complicated than that given in (22.4), but the conclusion about space-like correlations of near-field events still holds. Thus, with or without field–matter interaction, we shall prove in Sect. 24.3 that the *equal-time* commutator for $\mathbf{r} \neq \mathbf{r}'$ is given by

$$[\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}', t)] = \frac{\hbar}{i\epsilon_0} \delta_{\text{T}}(\mathbf{R}). \quad (22.5)$$

The presence of the transverse delta function, $\delta_{\text{T}}(\mathbf{R})$, shows that the fields of mesoscopic (and atomic) objects in rim-zone contact in general are correlated (also) outside the light cone.

22.3 Maxwell–Lorentz Operator Equations: Coulomb and Poincaré Gauges

In nonrelativistic QED field–matter interactions are most often are studied in the Coulomb gauge, where only the transverse part of the electromagnetic field is quantized. With a knowledge of the fully quantized Hamiltonian operator of the coupled particle–field system, or an adequate approximation for this operator, the temporal evolution of the global system is described starting from the Schrödinger, Heisenberg, or Interaction picture. In the Heisenberg picture the operators evolve in time but the state vector is fixed. The Heisenberg picture has the advantage that it is quite appropriate for comparisons between classical electrodynamics and QED, and this in itself makes this picture particularly useful for us.

In our classical (Part I) and semiclassical (Part II) studies in near-field electrodynamics we have seen the usefulness of electromagnetic propagator and Green function formalisms. Since these formalisms relate to integral equation formulations of the content of the Maxwell–Lorentz equations, it is of importance to know whether the form which the microscopic set of Maxwell–Lorentz equations has

among the classical field vectors and the material four-current density also holds for the associated operators. In order to study this one conveniently starts from the Heisenberg equation of motion for the general Heisenberg operator ($\hat{O}^H$), and with the Hamilton operator of the global field–particle system given in the Coulomb gauge. In Sect. 23.4 we show, beginning with the Heisenberg equations of motions for the field annihilation and creation operators belonging to a given plane-wave mode, that the dynamical equations for the $\hat{\mathbf{E}}_T$ - and $\hat{\mathbf{B}}$ -operators reproduce (in operator form) the transverse set of Maxwell–Lorentz equations ((9.25) and (9.26)). The longitudinal dynamics, given in a classical context by (9.27) and (9.28), is easily extended to the operator level, since the longitudinal electric field operator relates only to the particle position operators. Altogether, one comes to the conclusion that the Maxwell–Lorentz operator equations are form-identical to the corresponding classical equations *in the Coulomb gauge* [178, 180]. In other gauges the dynamical equations for the transverse field operators $\hat{\mathbf{E}}_T$ and $\hat{\mathbf{B}}$ will in general not be form-identical to the corresponding classical Maxwell–Lorentz equations [180].

In Sect. 10.4.1 we introduced generalized microscopic polarization and magnetization concepts, and afterwards these concepts were used in microscopic response theory (Sect. 10.5), in the formulation of microscopic electrodynamics based on $\mathbf{D}$ - and $\mathbf{H}$ -fields (Sect. 18.1), and in relation to a study of the photon embryo concept in photon wave mechanics (Sect. 18.2). In QED, a specific choice of the generalized polarization leads us to the form the Maxwell–Lorentz operator equations take in the Poincaré gauge, a useful gauge for the understanding of certain aspects of near-field QED.

The Coulomb and Poincaré gauges are closely related in the sense that the wave vector in the Coulomb (C) gauge is perpendicular to the wave vector everywhere in reciprocal space, and in the Poincaré (P) gauge it is perpendicular to the position vector everywhere in direct space, that is

$$\mathbf{q} \cdot \mathbf{A}^C(\mathbf{q}; t) = \mathbf{r} \cdot \mathbf{A}^P(\mathbf{r}, t) = 0. \quad (22.6)$$

The bridge between the quantum descriptions in the Coulomb and Poincaré gauges is a unitary transformation given by the operator [73, 178, 318–321]

$$\hat{T} = \exp \left(\frac{i}{\hbar} \sum_{\alpha} q_{\alpha} \hat{\chi}^P(\hat{\mathbf{r}}_{\alpha}) \right), \quad (22.7)$$

where $\hat{\chi}^P(\mathbf{r})$ is the gauge function for the C→P transformation. The summation is over the various particles of the system under study, $\hat{\mathbf{r}}_{\alpha}$ being the position operator of particle α . In the NEW (Poincaré) description the conjugate field position and momentum operators are $\hat{\mathbf{A}}_T^{\text{NEW}} = \hat{\mathbf{A}}_T$ and $\hat{\Pi}^{\text{NEW}} = -\hat{\mathbf{D}}^{\text{NEW}} = -\epsilon_0 \hat{\mathbf{E}}_T$, and altogether it turns out that the set of Maxwell–Lorentz operator equations in the Poincaré gauge becomes form-identical to the classical set expressed in terms of the microscopic vectors $\mathbf{D}$, $\mathbf{B}$, $\mathbf{P}_T$ and $\mathbf{M}$.

22.4 Covariant Field Propagators

After having studied Part I and Part II of this book the reader may have come to love and/or hate electromagnetic propagators and Green functions. Notwithstanding the fact that all phenomena in (near-field) electrodynamics can be treated without use of these, one cannot deny that the propagators (Green functions) provide us with an intuitively simple picture of the physical interaction between charged particles. Also, the great usefulness of propagators in practical near-field calculations is proven in numerous scientific publications. So, in Part III (Sects. 24.1, 24.4, 29.5, 30.1 and 30.2) the reader will meet more animals from the propagator zoo.

A number of important covariant scalar propagators are conveniently represented as contour integrals in a complex q^0 -plane, q^0 being the timely component of the covariant wave four-vector. Thus, the integral [155]

$$\Delta(x) = c_0 \int_C \frac{e^{-iq_\mu x^\mu}}{Q_C^2 - q_\mu q^\mu} \frac{d^4 q}{(2\pi)^4}, \quad (22.8)$$

where Q_C is the Compton wave number, can dependent on the contour (C) choice (and the direction of circulation) give us two important propagators, viz., the massive Jordan–Pauli propagator and the massive meson (Feynman) propagator [155]. Also, a valuable Huygens-like scalar propagator involving the analytical part of the Dirac delta function can be represented by (22.8). The commutator $[\hat{A}_T, \hat{E}_T]$, which is so important for an understanding of near-field correlations, is intimately related to the massless ($Q_C \rightarrow 0$) Jordan–Pauli propagator.

The meson propagator is of great importance in relativistic quantum field theory [155]. One reason for this stems from the fact that space-like separated events $[(x - x')^2 < 0]$ play a role in this theory. Thus, what constitutes “later” and what “earlier” depends on the frame of reference for $(x - x')^2 < 0$. In the meson propagator both cases are considered together. Since space-like separated events also are of importance in near-field electrodynamics a massless meson propagator description extended to the four-potential formalism of the photon necessarily must be of interest in a manifestly covariant theory for near-field interaction. Since the photon of course is a central quantity in relativistic quantum field theory, the relevant propagator already exist: The Feynman photon propagator. Perhaps, it is not surprising that the commutator $[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')]$ enters the covariant photon theory, and from what was said above, the time-ordered product (also called the T -product) $T\{\hat{A}^\mu(x)\hat{A}^\nu(x')\}$ surely must be of importance. The Feynman photon propagator is the quantum mechanical mean value of this T -product in the photon vacuum state. As we shall realize in Sect. 29.5.3, this mean value is given by

$$\langle 0|T\{\hat{A}^\mu(x)\hat{A}^\nu(x')\}|0\rangle = \frac{\hbar g^{\mu\nu}}{i\epsilon_0 c_0^2} \lim_{m \rightarrow 0} \Delta_F(x - x'), \quad (22.9)$$

$\Delta_F(x - x')$ being the meson scalar propagator. Roughly speaking, the Feynman photon propagator describes photon exchange between the space-time annihilation (x') and creation (x) points.

A contour integral representation along a certain contour allows one to pick out the contributions to the Feynman photon propagator from the longitudinal and scalar photons. A specific combination of the L - and S -contributions gives us the instantaneous Coulomb “propagator,” a quantity of particular interest in near-field electrodynamics.

To examine the connection between the Feynman photon propagator and the near-field and gauge photon formalism, it is convenient to make the covariant field quantization with an indefinite metric operator ($\hat{M}$). Such a quantization formalism can solve the difficulties associated with the negative norms appearing for states containing an odd-number of scalar photons. A complete systematic formalism in which states with negative norms do not appear has been developed by Gupta [314] and by Bleuler [315] (see also [236, 322, 323]), and elements of this formalism is briefly described in Sect. 29.4, paying particular attention to the near-field and gauge photons. In Sect. 30.1.2 we extend the Feynman photon propagator to the Gupta–Bleuler level, that is,

$$\subset 0|T\{\hat{A}^\mu(x)\hat{A}^\nu(x')\}|0 \supset = \langle 0|\hat{M}T\{\hat{A}^\mu(x)\hat{A}^\nu(x')\}|0\rangle. \quad (22.10)$$

Starting from the vacuum mean value in (22.10), it is possible to filter out from the associated momentum space propagator the near-field and gauge photon contributions.

We end our long journey with electromagnetic propagators (and Green functions) with a brief account of the so-called scattering propagator (Sect. 30.2.2). This covariant propagator, which, as its name indicates, is of particular interest for electromagnetic scattering problems, is just the difference between the retarded and advanced Huygens scalar propagators. Apart from a trivial constant the scattering propagator is identical to the massless Jordan–Pauli propagator.

22.5 Photon Emission from Atoms and Mesoscopic Objects

The emission of quantized radiation from micro- and mesoscopic particles is a subject of considerable interest in near-field QED. From the Heisenberg equation of motion for the photon annihilation operator $\hat{a}_{qs}(t)$, and with the nonrelativistic Hamilton operator of the fully quantized particle-system given in the Coulomb gauge, it is possible to derive an important integral relation between the transverse vector potential ($\hat{\mathbf{A}}_T(\mathbf{r}, t)$) and (source) current density ($\hat{\mathbf{J}}_T(\mathbf{r}, t)$) operators. The same integral relation also can be obtained directly from the Maxwell–Lorentz operator equations, taking the form they appear in using the Coulomb gauge. The kernel in the integral relation is just the Huygens scalar propagator. Two historically famous physical phenomena start to emerge from the integral equation, viz.,

the spontaneous emission [295, 324, 326] and the Lamb shift [157, 325–327]. Both of these phenomena may be considered as originating in the atom’s (mesoscopic particle’s) interaction with its own TRANSVERSE field. An alternative explanation of the spontaneous emission relates the process to the particle’s interaction with the vacuum fluctuations in the quantum field [329, 330]. An elaborate quantum electrodynamical calculation indicates that the two “physical pictures” (self-field, vacuum fluctuations) result in identical observational consequences [328]. In the self-field picture one assumes that the field retardation across the particle is small. Thus, if one expands the retarded transverse current density operator, $\hat{\mathbf{J}}_T(\mathbf{r}', t - |\mathbf{r} - \mathbf{r}'|/c_0)$ in a Taylor series around $\hat{\mathbf{J}}_T(\mathbf{r}', t)$ the first (non-retarded) term is associated to the spontaneous emission; see Sect. 27.1.1, and the neoclassical paper by Crisp and Jaynes [331]. In a near-field perspective, the two phenomena are somewhat different. Hence, the part of the transverse vector potential operator which relates to spontaneous emission involves an integral of $\hat{\mathbf{J}}_T(\mathbf{r}', t)$ over the near-field domain. This integral can be shown to equal the integral of $\hat{\mathbf{J}}(\mathbf{r}', t)$ over the atomic domain (the domain of nonvanishing electron density) multiplied by a factor $2/3$. For the Lamb shift the relevant quantity is the integral of $\hat{\mathbf{J}}_T(\mathbf{r}', t)/|\mathbf{r} - \mathbf{r}'|$ over the near-field domain. This integral cannot be reduced to an integral over just the atomic domain. The relation between $\hat{\mathbf{A}}_T$ and $\hat{\mathbf{J}}_T$ is gauge invariant because both these vector fields are the same in all gauges. The same relation, therefore, can be derived starting from say the Poincaré gauge. It must be noted, however, that the primary “electric” field operator is $\hat{\mathbf{D}}/\epsilon_0$ in the Poincaré gauge, and not $\hat{\mathbf{E}}_T$, and that the local source strength is $\nabla' \times (\nabla' \times \hat{\mathbf{P}} - c_0^{-2} \partial \hat{\mathbf{M}}/\partial t')$, and not $\hat{\mathbf{J}}_T$. Although the source region in the Poincaré gauge thus extends only over the atomic (or mesoscopic) domain, the advantage is counterbalanced by the fact that the connection between $\hat{\mathbf{D}}$ and $\hat{\mathbf{E}}_T$ is spatially nonlocal, yet timely local. The range of this nonlocality has the extension of the rim zone.

Qualitative insight in fundamental aspects of the photon emission process can be gained by theoretical studies of simplified models. In Sect. 27.2, we thus present a brief investigation of the field radiation from single-electron sources, i.e., sources where just one electron is electrodynamically active. The investigation gives us an opportunity to introduce the flip operator concept. Readers familiar with the second-quantization procedure for the electron wave-field (here the one-electron Schrödinger equation), will say that the flip operator belonging to the $i \rightarrow j$ transition describes a double process where one annihilates an electron in state i , and creates one in state j .

In studies of the photon emission from mesoscopic objects, one can in most cases neglect the variations of the transverse fields ($\mathbf{E}_T$, $\mathbf{B}$ and $\mathbf{A}_T$) across the objects, but of course not that of the longitudinal electric field, $\mathbf{E}_L$. This so-called long-wavelength approximation [53, 74, 178] is considered in Sect. 27.3, emphasizing the simplification it gives rise to in the Hamiltonian of the coupled field–particle system. The approximation is generally known as the electric dipole approximation because only the electric dipole moment of the source charge distribution enters the analysis. The celebrated electric dipole approximation is useful for a wide spectrum of analyses in classical electrodynamics and QED. Starting in the Poincaré gauge

we show that the electric dipole interaction Hamiltonian takes the form $\epsilon_0^{-1} \hat{\mathbf{d}} \cdot \hat{\mathbf{D}}$, where $\hat{\mathbf{d}}$ is the electric dipole moment operator of the charge system, and $\hat{\mathbf{D}}$ is the space-independent electric displacement field operator acting on the system. The electric dipole approximation simplifies the field–particle interaction enormously, as we shall realize later on. The particle part of the Hamiltonian gets an additional term in the electric dipole limit, viz., a term which gives the (infinite) self-energy of the electric dipoles in the system [178]. In a quantum electrodynamic context the electric dipole Hamiltonian may be derived from the general Coulomb Hamiltonian by subjecting this to a long-wavelength unitary transformation of the form

$$\hat{T} = \exp \left(-\frac{i}{\hbar} \hat{\mathbf{d}} \cdot \hat{\mathbf{A}}_{\text{T}}(\mathbf{0}) \right). \quad (22.11)$$

When (quasi-) monochromatic light interacts resonantly with a given pair of electronic levels it is sometimes possible to neglect the presence of all other levels. The atom (or mesoscopic particle) is thus treated as a two-level system [53, 74, 304, 305, 332–336]. In fundamental quantum optics, theoretical studies of the electric dipole interaction between a quantized electromagnetic field and a two-level system (e.g., an atom) is of central importance, and a number of fine books describe this kind of interaction in detail. In Sect. 27.4, we introduce and discuss the raising and lowering operators, the Pauli operators, and electron-field operators for a two-level system, and thereafter we set up the electric dipole Hamilton operator for the system. Finally, four fundamental physical processes entering the interaction Hamiltonian are described. In and near resonance two of these processes dominate the interaction, namely those satisfying (approximately) the energy conservation law. If only the two energy conserving interaction processes are kept we work in the so-called rotating-wave approximation (RW-approximation) [336].

The dynamical evolution of a two-level atom (mesoscopic particle) coupled to a quantized radiation field is conveniently described in terms of the Heisenberg equation of motions for (1) the atomic flip operator, plus (2) the field annihilation operators for the various field modes, ($\mathbf{q}_s$); see Sect. 27.5. In the RW-approximation this set of equations takes a quite simple form, yet not so simple that an exact analytical solution can be obtained. A qualitative description of the spontaneous emission process and the Lamb shift quite easily emerges if one makes the so-called Markov approximation [53, 305]. This approximation removes the timely nonlocality from the integro-differential equation for the atomic flip operator and in a sense, one may now claim that the dynamical evolution of the two-level dynamics is memory-less. Finally, we end up with expressions for the spontaneous decay rate and the *divergent* Lamb-shift operator. In a heuristic fashion it is outlined how the linear divergence of the Lamb-shift parameter at high frequencies can be reduced to a logarithmic divergence via a renormalization of the electron mass (from the bare mass of the experimentally observed mass). The renormalization is rooted in the electron’s electromagnetic interaction with its own field [178, 326, 327]. In a non-relativistic calculation the remaining divergence is removed by cutting the involved integral over frequency at the relativistic limit, $mc_0^2/\hbar$.

22.6 Virtual Transverse Photon Exchange in Near-Field Electrodynamics

In the Coulomb gauge, particles interact via instantaneous Coulomb forces and by exchange of transverse photons. In near-field QED, it is therefore important to study how the usually dominating Coulomb interaction is modified by the retarded exchange of photons. A qualitative analysis of the problem can be made by considering just two localized charge distributions A and B . To use the word “two” in a meaningful manner there must be no (essential) electronic spatial overlap between the quantum mechanical charge density distributions of A and B . From a quantum physical point of view a general analysis of the nonretarded Coulomb interaction between A and B constitutes a difficult problem in itself, and in order to elucidate the role of the transverse photon exchange, it is useful to simplify the expression for the Coulomb interaction energy somewhat. In near-field studies one often can assume that the spatial extension of each of the two charge distributions is small in comparison to the distance between them. Such an assumption usually is a good one in practical calculations of the interaction between mesoscopic (or microscopic) particles. With the assumption above the Coulomb interaction energy between A and B can be expanded in a certain multipole series, as described in Sect. 28.1. In powers of the reciprocal center of mass distance, R^{-1} , the leading term gives the Coulomb interaction energy between A and B ’s total charges. This term has a distance dependence R^{-1} . If only the leading term is kept the interaction is the same as between two charged point-particles. If at least one of the A and B ’s is electrically neutral the R^{-1} -term vanishes. The second term in the series is proportional to R^{-2} and describes the charge–dipole interaction between A and B . If both charge distributions are neutral this interaction vanishes. The third term, proportional to R^{-3} , accounts for the charge–quadrupole and dipole–dipole interactions between A and B . For neutral particle systems, the dipole–dipole interaction dominates the Coulomb interaction. This apparently instantaneous interaction process is a near-field phenomenon, which may be visualized as a quasi-static exchange of *virtual transverse photons*. As such the process is the so-called Van der Waals interaction [72, 73, 337, 338].

In Chap. 28, the single-photon exchange between two charged point particles and the Van der Waals interaction between two neutral particles are studied on the basis of perturbation theory with a so-called effective electronic Hamiltonian. A few qualitative considerations are devoted to the quantum theory of particle–surface interaction, the Casimir effect [73, 74, 339–344]. The exchange of a transverse photon gives rise to two corrections to the instantaneous Coulomb interaction between two point-particles, viz., a so-called delay correction and a magnetic correction. A good approach to the Van der Waals interaction can be obtained by looking at the process in the so-called Power–Zienau–Woolley representation of QED [73, 178, 318–320]. Essentially, this amounts to a study in an extended Poincaré gauge having two reference points, located conveniently at the center of masses for the A and B systems. In the Power–Zienau–Woolley description there

is no instantaneous interaction between A and B , and the near-field interaction between the two composite particles originates exclusively in the exchange of virtual transverse photons (photon embryos in the language of photon wave mechanics).

22.7 Exchange of Scalar Photons

In the covariant formulation of QED, the instantaneous Coulomb interaction between two point-particles appears to stem from an exchange of scalar and longitudinal photons [178]. Perhaps, this is not surprising for the reader because it has been indicated in Sect. 22.5 that the Coulomb part of the Feynman photon propagator is obtained by a combination of the longitudinal and scalar photon contributions to the photon propagator. In the simple case where the two point-charges are fixed in space only scalar photons are exchanged. The global ground state of the field is the photon vacuum. By placing two fixed charges in the otherwise free space, the ground state energy of the field is modified by scalar photon exchange. The energy change is precisely the Coulomb energy of the particles. Single-photon exchange basically is sufficient to reach this conclusion. The Coulomb interaction energy appears as stemming from two processes: (1) A scalar photon emission from A followed by an absorption of this photon in B , and (2) the inverse process. The Coulomb self-energy of say particle A originates in emission and reabsorption of a scalar photon by A . To obtain the entire Coulomb energy of the two particles a summation must be made over the entire q -spectrum of scalar photons. In the near-field and gauge photon picture it turns out that only the *displaced* ground state of the near-field oscillators is of importance for the Coulomb interaction. In consequence, the Coulomb interaction can be calculated via exchange of gauge photons. All physical states involved in the interaction are coherent states of the original (undisplaced) scalar (or near-field) photon field.

22.8 Coherent States of Evanescent Fields

We know from the analysis in Chap. 4 that the angular spectrum representation of classical electromagnetic fields plays an important role in near-field studies of the radiative and nonradiative fields generated by sheet sources and plane structure sources (surfaces, interfaces, and layered media). In a quantum electrodynamic description the nonradiative (evanescent) fields are related *primarily* to the longitudinal and scalar photons, but also to virtual transverse photons. As a forerunner to a brief discussion of the coherent scalar and longitudinal photon emission from a sheet source, we calculate in Sect. 30.5 the classical longitudinal and scalar potentials generated by a sheet carrying a prescribed current density distribution. A knowledge of these potentials in the quasi-static limit allows one to determine the rim zone of the sheet. A prescribed mean current density without significant quantum fluctuations

we call a classical current density. With a prescribed classical current density it is quite simple to solve the Heisenberg equations of motions for the annihilation operators belonging to the longitudinal and scalar photon fields, and thereafter show that the quantum states of these fields are coherent states [53, 74, 178, 305, 345–350]. A coherent state, which is an eigenstate for the annihilation operator of the given mode, is characterized by a complex number. As a function of the field wave vector (and of time), this number is called the complex coherence function. In Sect. 30.6.4 we calculate the coherence functions for the longitudinal and scalar photon states.

Chapter 23

The Route to the Maxwell–Lorentz Operator Equations in the Coulomb Gauge

23.1 Plane-Wave Quantization of the Transverse Electromagnetic Field

In the present section, a brief review of certain (a few) aspects of the standard theory for quantization of the transverse degrees of freedom of the electromagnetic field is given. For a more rigorous and detailed account the reader is urged to consult e.g., [178].

23.1.1 *The Classical Field Vectors*

It is common to consider the electromagnetic field as being confined in an enclosure (closed or open). Such a starting point certainly is physically appealing if one aims at studying quantum electrodynamic phenomena in simple cavities, e.g., an atom interacting with an electromagnetic field in a superconducting (or metallic) cavity. In such problems it is important to seek to subject the electromagnetic field to the correct boundary conditions at the faces of the cavity. In general the establishment of these conditions involves a complicated calculation of the field–matter interaction in the boundary region [21, 85, 351–355]. Rigorously speaking, the electromagnetic field can never from a microscopic point of view vanish exactly at a boundary. A sharp boundary for the field is an abstraction. The field will always possess some kind of “tail” outside the cavity. Whether or not it is necessary to solve the boundary problem in detail depends on the subject under investigation. In a number of important cases it is sufficient to use the standard (textbook) boundary conditions [19].

Outside the field of cavity quantum electrodynamics it is also useful to assume that the field is confined to a certain region of space. For simplicity, it is here assumed that the enclosure is a large cube of edge L . Inside the cube a given field vector can then be represented as a Fourier series, i.e., it is specified by a denumerable set of Fourier expansion coefficients. If our unphysical cube is sufficiently large all physical predictions will be independent of L , and of the chosen set of

boundary conditions. It is not necessary to confine the field in an imaginary cavity. The quantization procedure for the electromagnetic field can be carried out also in an infinite space domain. In infinite space the electromagnetic field possesses a continuous infinity of degrees of freedom, and in the limit $L \rightarrow \infty$ this also will be the case for a field confined to a fictitious cube. Thus, for $L \rightarrow \infty$ any discrete sum over Fourier ($\mathbf{q}$) vectors becomes an integral according to the rule

$$L^{-3} \sum_{\mathbf{q}} (\dots) \rightarrow (2\pi)^{-3} \int_{-\infty}^{\infty} (\dots) d^3 q. \quad (23.1)$$

If the cube is placed with its edges along the Cartesian axes of an (x, y, z) -coordinate system, and we choose the well known periodic boundary conditions for the various field vectors, the Fourier vector can take on only one of the discrete values

$$\mathbf{q} = \frac{2\pi}{L} (n_x, n_y, n_z), \quad n_x, n_y, n_z = 0, \pm 1, \pm 2, \dots \quad (23.2)$$

We can now expand the transverse vector potential $\mathbf{A}_T(\mathbf{r}, t)$ in a Fourier series

$$\mathbf{A}_T(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q}} (\mathbf{A}_{T,\mathbf{q}}(t) e^{i\mathbf{q} \cdot \mathbf{r}} + c.c.). \quad (23.3)$$

The form of the series in (23.3) ensures that the potential is a real quantity. The reality of $\mathbf{A}_T(\mathbf{r}, t)$ implies that

$$\mathbf{A}_{T,-\mathbf{q}}(t) = \mathbf{A}_{T,\mathbf{q}}^*(t), \quad (23.4)$$

as the reader may verify. The transversality of the vector potential is expressed through

$$\mathbf{q} \cdot \mathbf{A}_{T,\mathbf{q}}(t) = 0, \quad (23.5)$$

an equation which must hold for all $\mathbf{q}$ -vectors. For each $\mathbf{q}$ -direction, we introduce a set of three mutually perpendicular real unit vectors according to the conditions in (15.49)–(15.51). The unit vectors are designated by $\boldsymbol{\kappa} = \mathbf{q}/q$, ϵ_{q1} and ϵ_{q2} , and to avoid confusion with the operator symbol $\wedge$ unit vectors are written without a caret in this part of the book. The transversality condition in (23.5) allows one to expand $\mathbf{A}_{T,\mathbf{q}}(t)$ after the unit vectors $\epsilon_{q,s}$ ($s = 1, 2$). Thus,

$$\mathbf{A}_{T,\mathbf{q}}(t) = \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \sum_{s=1}^2 \alpha_{qs}(t) \epsilon_{qs}, \quad (23.6)$$

where $\omega_q = c_0 q$. The usefulness in separating off a factor $[\hbar/(2\epsilon_0 \omega_q)]^{1/2}$ will become clear when we express the energy of the transverse part of the electromagnetic field in terms of the amplitudes of the Fourier series for the transverse vector potential. From the decomposition

$$A_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0\omega_q} \right)^{1/2} \boldsymbol{\epsilon}_{q,s} (\alpha_{qs}(t) e^{i\mathbf{q}\cdot\mathbf{r}} + c.c.), \quad (23.7)$$

and (9.39) and (9.40), the following plane-mode expansions are obtained for the transverse electric and magnetic fields:

$$\mathbf{E}_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0\omega_q} \right)^{1/2} \boldsymbol{\epsilon}_{qs} \left(-\frac{d}{dt} \alpha_{qs}(t) e^{i\mathbf{q}\cdot\mathbf{r}} + c.c. \right), \quad (23.8)$$

$$\mathbf{B}(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar\omega_q}{2\epsilon_0 c_0^2} \right)^{1/2} \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} (i\alpha_{qs}(t) e^{i\mathbf{q}\cdot\mathbf{r}} + c.c.). \quad (23.9)$$

The transverse dynamics must satisfy (9.26), or equivalently (9.35). If one inserts (23.8), (23.9), and the plane-mode expansion for the transverse current density, viz.,

$$\mathbf{J}_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} (\boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} \cdot \mathbf{J}_{T,q}(t) e^{i\mathbf{q}\cdot\mathbf{r}} + c.c.) \quad (23.10)$$

into (9.26), one obtains, as the reader may show, the following second-order differential equation for the mode amplitude α_{qs} :

$$\left(\frac{d^2}{dt^2} + \omega_q^2 \right) \alpha_{qs}(t) = \left(\frac{2\omega_q}{\hbar\epsilon_0} \right)^{1/2} \boldsymbol{\epsilon}_{qs} \cdot \mathbf{J}_{T,q}(t). \quad (23.11)$$

On the right-hand side of this equation appears the projection of the Fourier amplitude of the transverse current density, $\mathbf{J}_{T,q}(t)$, on the direction given by the unit vector $\boldsymbol{\epsilon}_{qs}$.

In free space α_{qs} satisfies the homogeneous differential equation

$$\left(\frac{d^2}{dt^2} + \omega_q^2 \right) \alpha_{qs}(t) = 0. \quad (23.12)$$

The general solution to this equation may be written as a linear combination of solutions of the types $\exp(\pm i\omega_q t)$. The “positive-frequency” solution

$$\alpha_{qs}(t) = \alpha_{qs}(0) e^{-i\omega_q t} \quad (23.13)$$

leads, when inserted into (23.7), to the following monochromatic plane-wave expansion of the vector potential in free space:

$$A_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0\omega_q} \right)^{1/2} \boldsymbol{\epsilon}_{qs} \left[\alpha_{qs}(0) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_q t)} + c.c. \right]. \quad (23.14)$$

Nothing extra is obtained by choosing the “negative-frequency” solution. The reader may convince himself of this making the replacement $\mathbf{q} \Rightarrow -\mathbf{q}$ in (23.7). With $\alpha_{qs}(t)$ given by (23.13) the expansions of the electric and magnetic free-space fields become

$$\mathbf{E}_T(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q}, s} \left(\frac{\hbar \omega_q}{2\epsilon_0} \right)^{1/2} \boldsymbol{\epsilon}_{qs} \left[i\alpha_{qs}(0) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_q t)} + c.c. \right], \quad (23.15)$$

$$\mathbf{B}(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q}, s} \left(\frac{\hbar \omega_q}{2\epsilon_0 c_0^2} \right)^{1/2} \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} \left[i\alpha_{qs}(0) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_q t)} + c.c. \right]. \quad (23.16)$$

23.1.2 The Classical Field Energy and Momentum in Free Space

We shall see now that it is possible to express the energy in the free electromagnetic field solely in terms of the set of normal mode amplitudes, $\alpha_{qs}(0)$. To achieve this goal one inserts (23.15) and (23.16) into (9.70). The energy H_{trans} is in this part of the book denoted by H_F , where the subscript F stands for (radiation) field. After some simple algebra one obtains

$$\begin{aligned} H_F = & \frac{\hbar}{4} \sum_{\mathbf{q}, s} \sum_{\mathbf{q}', s'} \{ (\omega_q \omega_{q'})^{1/2} [\boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{q's'} + (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot (\boldsymbol{\kappa}' \times \boldsymbol{\epsilon}_{q's'})] \\ & \times L^{-3} \int_V (i\alpha_{qs}(t) e^{i\mathbf{q} \cdot \mathbf{r}} + c.c.) (i\alpha_{q's'}(t) e^{i\mathbf{q}' \cdot \mathbf{r}} + c.c.) d^3 r \}, \end{aligned} \quad (23.17)$$

where $\alpha_{qs}(t)$ is given by (23.13). The integration over the cavity volume $V (= L^3)$ is at once carried out by means of the formulas

$$L^{-3} \int_V e^{\pm i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{r}} d^3 r = \delta_{\mathbf{q}, -\mathbf{q}'}, \quad (23.18)$$

$$L^{-3} \int_V e^{\pm i(\mathbf{q} - \mathbf{q}') \cdot \mathbf{r}} d^3 r = \delta_{\mathbf{q}, \mathbf{q}'}. \quad (23.19)$$

The appearance of the Kronecker delta's in turn allows one to eliminate the summation over $\mathbf{q}'$ in (23.17). Hence, one gets

$$\begin{aligned} H_F = & \frac{\hbar}{4} \sum_{\mathbf{q}, s, s'} \omega_q \{ - [\boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{-qs'} + (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot (-\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{-qs'})] \\ & \times (\alpha_{qs}(t) \alpha_{-qs'}(t) + \alpha_{qs}^*(t) \alpha_{-qs'}^*(t)) [\boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{qs'} + (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs'})] \\ & + (\alpha_{qs}(t) \alpha_{qs'}^*(t) + \alpha_{qs}^*(t) \alpha_{qs'}(t)) \}. \end{aligned} \quad (23.20)$$

Since

$$(\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot (-\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{-qs'}) = \boldsymbol{\kappa} \times (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot \boldsymbol{\epsilon}_{-qs'} = -\boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{-qs'}, \quad (23.21)$$

and therefore

$$(\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}) \cdot (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs'}) = \boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{qs'} = \delta_{s,s'}, \quad (23.22)$$

one finally obtains

$$H_F = \sum_{q,s} \frac{\hbar \omega_q}{2} \left(\alpha_{qs}^*(t) \alpha_{qs}(t) + \alpha_{qs}(t) \alpha_{qs}^*(t) \right), \quad (23.23)$$

or equivalently

$$H_F = \sum_{q,s} \hbar \omega_q \alpha_{qs}^*(t) \alpha_{qs}(t). \quad (23.24)$$

The energy in the free electromagnetic field thus appears as the sum of the energies of a set of fictitious uncoupled harmonic oscillators (modes). There is an oscillator associated with each pair of vectors $\mathbf{q}$, $\boldsymbol{\epsilon}_{qs}$, and the oscillator frequency is $\omega_q = c_0 q$. The oscillator frequency depends on the magnitude of $\mathbf{q}$, but not its direction. The free-field energy H_F is of course independent of time, and this fact becomes manifest if one inserts (23.13) and its complex conjugate into (23.24). Thus,

$$H_F = \sum_{q,s} \hbar \omega_q \alpha_{qs}^*(0) \alpha_{qs}(0). \quad (23.25)$$

The momentum of the free electromagnetic field, $\mathbf{P}_{\text{trans}} \equiv \mathbf{P}_F$, can also be expressed as a sum of momenta belonging to the various running modes. By inserting (23.15) and (23.16) into (9.81), and making use of (23.18) and (23.19), we obtain

$$\begin{aligned} \mathbf{P}_F = & \frac{1}{2} \sum_{q,s,s'} \frac{\hbar \omega_q}{c_0} \left[\boldsymbol{\epsilon}_{qs} \times (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{-qs'}) \left(\alpha_{qs}(t) \alpha_{-qs'}(t) + \alpha_{qs}^*(t) \alpha_{-qs'}^*(t) \right) \right. \\ & \left. + \boldsymbol{\epsilon}_{qs} \times (\boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs'}) \left(\alpha_{qs}(t) \alpha_{qs'}^*(t) + \alpha_{qs}^*(t) \alpha_{qs'}(t) \right) \right], \end{aligned} \quad (23.26)$$

and then

$$\begin{aligned} \mathbf{P}_F = & \frac{1}{2} \sum_{q,s} \hbar \mathbf{q} \left(\alpha_{qs}^*(t) \alpha_{qs}(t) + c.c. \right) \\ & + \frac{1}{2} \sum_{q,s,s'} \hbar \mathbf{q} \left(\alpha_{qs}(t) \alpha_{-qs'}(t) + c.c. \right) \boldsymbol{\epsilon}_{qs} \cdot \boldsymbol{\epsilon}_{-qs'}. \end{aligned} \quad (23.27)$$

The last triple sum vanishes identically. The reader may prove this by adding the terms containing $\mathbf{q}$ and $-\mathbf{q}$ and interchanging in the terms with $-\mathbf{q}$ the dummy indices s and s' . Altogether, one thus ends up with

$$P_F = \sum_{\mathbf{q},s} \frac{\hbar \mathbf{q}}{2} \left(\alpha_{\mathbf{q}s}^*(t) \alpha_{\mathbf{q}s}(t) + \alpha_{\mathbf{q}s}(t) \alpha_{\mathbf{q}s}^*(t) \right) = \sum_{\mathbf{q},s} \hbar \mathbf{q} \alpha_{\mathbf{q}s}^*(t) \alpha_{\mathbf{q}s}(t), \quad (23.28)$$

a result which written in the form

$$P_F = \sum_{\mathbf{q},s} \hbar \mathbf{q} \alpha_{\mathbf{q}s}^*(0) \alpha_{\mathbf{q}s}(0) \quad (23.29)$$

manifestly shows that the momentum of the free field is independent of time.

23.1.3 The Classical Spin of the Free Field

Starting from (9.95) it is possible also to express the angular momentum of the free field as a sum of the angular momenta of the individual running modes. The mode expansion of the orbital part of the field momentum (17.23) is not needed in the remaining part of the book, and we shall therefore confine ourselves here to the expansion of the intrinsic (spin) part (17.24), which below is denoted by $\mathbf{S}_F$.

By inserting the expansions in (23.14) and (23.15) into (17.24), carrying out the integration over the cavity volume with the help of (23.18) and (23.19), and eliminating the summation over $\mathbf{q}'$ by means of the Kronecker delta's $\delta_{\mathbf{q},-\mathbf{q}'}$ and $\delta_{\mathbf{q},\mathbf{q}'}$, one obtains the intermediate result

$$\begin{aligned} \mathbf{S}_F = & \frac{\hbar}{2} \sum_{\mathbf{q},s,s'} \left[\boldsymbol{\epsilon}_{\mathbf{q}s} \times \boldsymbol{\epsilon}_{-\mathbf{q}s'} \left(i \alpha_{\mathbf{q}s}(t) \alpha_{-\mathbf{q}s'}(t) + c.c. \right) \right. \\ & \left. + \boldsymbol{\epsilon}_{\mathbf{q}s} \times \boldsymbol{\epsilon}_{\mathbf{q}s'} \left(i \alpha_{\mathbf{q}s}(t) \alpha_{\mathbf{q}s'}^*(t) + c.c. \right) \right]. \end{aligned} \quad (23.30)$$

The part containing the indices $(\mathbf{q}s)$ and $(-\mathbf{q}s')$ vanishes with the same argumentation as we used above (23.28) in the calculation of the field momentum. Hence, the expression for $\mathbf{S}_F$ is reduced to

$$\mathbf{S}_F = \frac{\hbar}{2} \sum_{\mathbf{q},s,s'} \boldsymbol{\epsilon}_{\mathbf{q}s} \times \boldsymbol{\epsilon}_{\mathbf{q}s'} \left(i \alpha_{\mathbf{q}s}(t) \alpha_{\mathbf{q}s'}^*(t) + c.c. \right). \quad (23.31)$$

The s' -summation can be eliminated by utilizing that

$$\boldsymbol{\epsilon}_{\mathbf{q}s} \times \boldsymbol{\epsilon}_{\mathbf{q}s'} = \pm \kappa (1 - \delta_{s,s'}), \quad (23.32)$$

where the upper and lower signs in front of κ correspond to $s = 1$ and 2, respectively. Thus, with the remaining summation over s carried out, one finally obtains

$$\mathbf{S}_F = i\hbar \sum_{\mathbf{q}} \kappa \left(\alpha_{q2}^*(t) \alpha_{q1}(t) - c.c. \right). \quad (23.33)$$

The result in (23.33) is not quite satisfactory because in each $\mathbf{q}$ -contribution the two linear polarization states are coupled. The reader may have anticipated this coupling due to the fact that the helicity states are the eigenstates for the photon's intrinsic angular momentum.

Let us therefore expand the Fourier amplitude $A_{T,\mathbf{q}}(t)$ after the (complex) helicity unit vectors $\mathbf{e}_{q+}$ and $\mathbf{e}_{q-}$, given (in a slightly different notation) in terms of the real polarization unit vectors in (15.53) and (15.54). With

$$A_{T,\mathbf{q}}(t) = \left(\frac{\hbar}{2\epsilon_0\omega_{\mathbf{q}}} \right)^{1/2} \sum_{s=+,-} \alpha_{qs}(t) \mathbf{e}_{qs}, \quad (23.34)$$

the transverse vector potential has the following monochromatic plane-wave expansion in free space:

$$\mathbf{A}_T(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q},s} \left(\frac{\hbar}{2\epsilon_0\omega_{\mathbf{q}}} \right)^{1/2} \left[\mathbf{e}_{qs} \alpha_{qs}(0) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)} + c.c. \right]. \quad (23.35)$$

By means of this expansion and an analogous one for $\mathbf{E}_T(\mathbf{r}, t)$, the spin of the free field can be calculated as above, remembering that the polarization unit vectors now are complex quantities. Instead of (23.31) one obtains

$$\mathbf{S}_F = \frac{\hbar}{2} \sum_{\mathbf{q},s,s'} \left(i \mathbf{e}_{qs} \times \mathbf{e}_{qs'}^* \alpha_{qs}(t) \alpha_{qs'}(t) + c.c. \right), \quad (23.36)$$

with the $\alpha_{qs}(t)$'s given by (23.13), as the reader may verify. By means of (15.51), (15.53) and (15.54), it is easy to prove that

$$\mathbf{e}_{qs} \times \mathbf{e}_{qs'} = -i\lambda_s \kappa \delta_{s,s'}, \quad (23.37)$$

where $\lambda_+ = +1$ and $\lambda_- = -1$. This result shows that the two helicity states are not coupled in a given $\mathbf{q}$ -mode. By inserting (23.37) into (23.36) one obtains

$$\mathbf{S}_F = \sum_{\mathbf{q}} \hbar \kappa \left(|\alpha_{q+}(0)|^2 - |\alpha_{q-}(0)|^2 \right). \quad (23.38)$$

The spin of the free field is time invariant, and for a given $\mathbf{q}$ the contributions to $\mathbf{S}_F$ from the positive- and negative-helicity components are parallel and antiparallel to κ , respectively. This is of course in agreement with the result obtained in the wave mechanical treatment of the photon spin in Chap. 17.

23.1.4 Quantization Scheme for the Radiation Field: Transverse Field Observables

The normal variables $\alpha_{qs}(0)$ and $\alpha_{qs}^*(0)$, which characterize the state of the classical free (transverse) electromagnetic field, we now replace by quantum operators, i.e.,

$$\alpha_{qs}(0) \Rightarrow \hat{a}_{qs}(0), \quad (23.39)$$

$$\alpha_{qs}^*(0) \Rightarrow \hat{a}_{qs}^\dagger(0), \quad (23.40)$$

and we then require that these operators satisfy the commutator relations

$$[\hat{a}_{qs}(0), \hat{a}_{q's'}(0)] = [\hat{a}_{qs}^\dagger(0), \hat{a}_{q's'}^\dagger(0)] = 0, \quad (23.41)$$

$$[\hat{a}_{qs}(0), \hat{a}_{q's'}^\dagger(0)] = \delta_{q,q'}\delta_{s,s'}. \quad (23.42)$$

The operators $\hat{a}_{qs}$ and $\hat{a}_{qs}^\dagger$ become the destruction (annihilation) and creation operators, respectively, for the fictitious harmonic oscillators associated with the various modes of the field. The requirements above originate in an extension of the quantum theory for the massive harmonic oscillator. For such an oscillator, destruction ($\hat{a}$) and creation ($\hat{a}^\dagger$) operators satisfying the commutation relation $[\hat{a}, \hat{a}^\dagger] = 1$ appear, as is well known from elementary quantum mechanics. For consistency with (23.13), the destruction and creation operators must for the *free electromagnetic field* involve in time according to

$$\hat{a}_{qs}(t) = \hat{a}_{qs}(0)e^{-i\omega_q t}, \quad (23.43)$$

$$\hat{a}_{qs}^\dagger(t) = \hat{a}_{qs}^\dagger(0)e^{i\omega_q t}, \quad (23.44)$$

in the Heisenberg picture (see Sect. 23.2). It is easy to prove that the operators $\hat{a}_{qs}(t)$ and $\hat{a}_{qs}^\dagger(t)$ satisfy commutator relations analogous to those given in (23.41) and (23.42).

It is now postulated that generalized quantum destruction ($\hat{a}_{qs}(t)$) and creation ($\hat{a}_{qs}^\dagger(t)$) operators, satisfying the *equal-time* commutator relations

$$[\hat{a}_{qs}(t), \hat{a}_{q's'}(t)] = [\hat{a}_{qs}^\dagger(t), \hat{a}_{q's'}^\dagger(t)] = 0, \quad (23.45)$$

$$[\hat{a}_{qs}(t), \hat{a}_{q's'}^\dagger(t)] = \delta_{q,q'}\delta_{s,s'}, \quad (23.46)$$

characterize (in the Heisenberg picture) the quantum state of the transverse electromagnetic field *even* in the presence of matter (charges). Since we know from the analysis in Chap. 9 that the classical state of a global field–particle system is completely characterized at a given time by the transverse part of the electromagnetic field at all space points ($\mathbf{r}$) plus the position and velocities of all particles

(cf. the specifications in (9.97)), the extended heuristic postulate may appear reasonable. A more satisfactory approach giving a deeper understanding important for quantum field theory as such is based on a Lagrangian and Hamiltonian approach. In this approach the Maxwell–Lorentz equations appear in the form of Lagrange equations derived variationally from a certain Lagrangian. Canonical quantization of the system is obtained by associating operators with commutator $i\hbar$ to each pair of “generalized coordinate” and associated “canonically conjugate momentum.”

In our framework (quantum electrodynamics), the conjugate position and momentum operators of the individual massive particles still are postulated to satisfy the commutator relations in (11.96) and (11.97).

Let us now consider the operators associated with the transverse fields, viz., $\hat{\mathbf{E}}_{\text{T}}$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{A}}_{\text{T}}$. In quantum physics, the time evolution of a system can be described in various pictures; see Sect. 23.2. In the Schrödinger picture, the operators are fixed in time, whereas they involve in time in the Heisenberg picture. We begin in the Schrödinger picture, and in Sect. 23.2 the time evolution of the various field operators are studied in the Heisenberg picture. With the replacements $\alpha_{qs} \rightarrow \hat{a}_{qs}$ and $\alpha_{qs}^* \rightarrow \hat{a}_{qs}^\dagger$, the transverse vectorial potential operator becomes

$$\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \left(\hat{a}_{qs} e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{a}_{qs}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \boldsymbol{\epsilon}_{qs}, \quad (23.47)$$

and the magnetic field operator is given by

$$\hat{\mathbf{B}}(\mathbf{r}) = L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0 c_0^2} \right)^{1/2} \left(\hat{a}_{qs} e^{i\mathbf{q} \cdot \mathbf{r}} - \hat{a}_{qs}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs}. \quad (23.48)$$

These Schrödinger picture operators are obtained from (23.7) and (23.9), remembering that $\hat{a}_{qs}$ and $\hat{a}_{qs}^\dagger$ here are time independent. One cannot translate the classical expression given in (23.8) for the transverse electric field to operator form in the Schrödinger picture, but since the operators are time independent in this picture one may start from the free-field formula for $\mathbf{E}_{\text{T}}$, leaving out the $\exp(-i\omega t)$ factor. Such a produce is expected to be correct since the field–matter interaction in all cases only exists over a finite time interval. Additional remarks on the extension of $\mathbf{E}_{\text{T}}$ to the operator level are given in Sect. 23.2. To the transverse electric field one hence associates the operator

$$\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}) = L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0} \right)^{1/2} \left(\hat{a}_{qs} e^{i\mathbf{q} \cdot \mathbf{r}} - \hat{a}_{qs}^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \boldsymbol{\epsilon}_{qs} \quad (23.49)$$

in the Schrödinger picture. The operators $\hat{\mathbf{A}}_{\text{T}}(\mathbf{r})$, $\hat{\mathbf{B}}(\mathbf{r})$ and $\hat{\mathbf{E}}_{\text{T}}(\mathbf{r})$ all are Hermitian.

23.1.5 *Hamilton, Momentum and Spin Operators for the Transverse Electromagnetic Field*

The global operator variable associated to the Hamiltonian of the transverse field (H_F) is obtained from (23.23). In the derivation of this equation from (9.70), the ordering of α_{qs} and α_{qs}^* has been respected, and it is therefore not necessary to redo these calculations in the quantum case starting from (23.48) and (23.49). In the Schrödinger picture the Hamilton operator of the transverse electromagnetic field, therefore, can be written in the form

$$\begin{aligned}\hat{H}_F &= \frac{\epsilon_0}{2} \int_V \left(\hat{\mathbf{E}}_T^2(\mathbf{r}) + \hat{\mathbf{B}}^2(\mathbf{r}) \right) d^3r \\ &= \sum_{q,s} \frac{\hbar\omega_q}{2} \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \hat{a}_{qs} \hat{a}_{qs}^\dagger \right),\end{aligned}\quad (23.50)$$

or as follows

$$\hat{H}_F = \sum_{q,s} \hbar\omega_q \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \frac{1}{2} \right), \quad (23.51)$$

as one realizes using the commutator relation $[\hat{a}_{qs}, \hat{a}_{qs}^\dagger] = 1$.

The global momentum operator for the transverse field follows from a translation of (23.28). Thus, one has

$$\begin{aligned}\hat{\mathbf{P}}_F &= \epsilon_0 \int_V \hat{\mathbf{E}}_T(\mathbf{r}) \times \hat{\mathbf{B}}(\mathbf{r}) d^3r \\ &= \sum_{q,s} \frac{\hbar\mathbf{q}}{2} \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \hat{a}_{qs} \hat{a}_{qs}^\dagger \right)\end{aligned}\quad (23.52)$$

in the Schrödinger picture. Since

$$\sum_{q,s} \frac{\hbar\mathbf{q}}{2} = \mathbf{0}, \quad (23.53)$$

$\hat{\mathbf{P}}_F$ can be written also in the more compact form

$$\hat{\mathbf{P}}_F = \sum_{q,s} \hbar\mathbf{q} \hat{a}_{qs}^\dagger \hat{a}_{qs}. \quad (23.54)$$

It follows from the analysis to be given in Chap. 24 that the operators $\hat{\mathbf{E}}_T(\mathbf{r})$ and $\hat{\mathbf{B}}(\mathbf{r})$ commute when they are taken at the same point. This fact makes it unnecessary to symmetrize the vector product $\hat{\mathbf{E}}_T(\mathbf{r}) \times \hat{\mathbf{B}}(\mathbf{r})$ in order to obtain a Hermitian from of the integral for the momentum (23.52). The expression given in (23.54) for $\hat{\mathbf{P}}_F$ is clearly Hermitian, and this confirms our conclusion, subsequently.

It appears from (23.38) that the spin operator of the transverse electromagnetic field in the helicity unit vector basis will be given by

$$\hat{S}_F = \sum_{\mathbf{q}} \hbar \kappa \left(\hat{a}_{\mathbf{q}+}^\dagger \hat{a}_{\mathbf{q}+} - \hat{a}_{\mathbf{q}-}^\dagger \hat{a}_{\mathbf{q}-} \right), \quad (23.55)$$

where $\hat{a}_{\mathbf{q}+}$ ($\hat{a}_{\mathbf{q}-}$) and $\hat{a}_{\mathbf{q}+}^\dagger$ ($\hat{a}_{\mathbf{q}-}^\dagger$) are the destruction and creation operators for the positive (negative) helicity modes in the Schrödinger picture.

23.1.6 Monochromatic Plane-Wave Photons: A Brief Review

In order to determine the eigenstates of the total energy and total momentum let us first consider one of the fictitious harmonic oscillators associated with the transverse field, and let us for brevity omit the subscripts $\mathbf{q}, s$ on the various quantities. Expressed in terms of the Hermitian number operator

$$\hat{N} \equiv \hat{a}^\dagger \hat{a}, \quad (23.56)$$

the radiation Hamiltonian is

$$\hat{H} = \hbar \omega \left(\hat{N} + \frac{1}{2} \right). \quad (23.57)$$

Since, for any quantum state $|\psi\rangle$

$$\langle \psi | \hat{N} | \psi \rangle = \langle \psi | \hat{a}^\dagger \hat{a} | \psi \rangle = \langle a \psi | a \psi \rangle \geq 0, \quad (23.58)$$

the number operator possesses a lowest non-negative eigenvalue $\beta_0 \geq 0$. It follows from the eigenvalue equation

$$\hat{N} |\beta\rangle = \beta |\beta\rangle, \quad (23.59)$$

and the commutator relation $[\hat{a}, \hat{a}^\dagger] = 1$ that

$$\hat{N} \hat{a} |\beta\rangle = (\hat{a} \hat{a}^\dagger - 1) \hat{a} |\beta\rangle = (\beta - 1) \hat{a} |\beta\rangle, \quad (23.60)$$

and

$$\hat{N} \hat{a}^\dagger |\beta\rangle = \hat{a}^\dagger (\hat{a}^\dagger \hat{a} + 1) |\beta\rangle = (\beta + 1) \hat{a}^\dagger |\beta\rangle. \quad (23.61)$$

The states $\hat{a} |\beta\rangle$ and $\hat{a}^\dagger |\beta\rangle$ therefore also are eigenfunctions of the number operator belonging to the eigenvalues $\beta - 1$ and $\beta + 1$, respectively. Since β_0 is the lowest eigenvalue one must have

$$\hat{a} |\beta_0\rangle = 0. \quad (23.62)$$

The quantum state $|\beta_0\rangle$ is called the ground state of the oscillator. From the eigenvalue equation for $\hat{N}$ one has

$$\hat{a}^\dagger \hat{a} |\beta_0\rangle = \beta_0 |\beta_0\rangle, \quad (23.63)$$

and together (23.62) and (23.63) implies $\beta_0 = 0$. The eigenvalues of the number operator thus are the integers $n = 0, 1, 2, \dots$. To emphasize this, the various eigenstates of $\hat{N}$ from now on are denoted by $|n\rangle$. In the new notation

$$\hat{a}^\dagger \hat{a} |n\rangle = n |n\rangle, \quad n = 0, 1, 2, \dots \quad (23.64)$$

The reader may verify himself that if the eigenvector $|n\rangle$ is normalized, i.e., $\langle n|n\rangle = 1$, the states $|n \pm 1\rangle$ will also be normalized provided

$$\hat{a} |n\rangle = n^{1/2} |n-1\rangle, \quad (23.65)$$

$$\hat{a}^\dagger |n\rangle = (n+1)^{1/2} |n+1\rangle. \quad (23.66)$$

Starting from the ground state $|0\rangle$, which we assume has been normalized ($\langle 0|0\rangle = 1$), it appears from (23.66) that various normalized eigenvectors of the number operator can be generated from the ground state as follows:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle, \quad n = 0, 1, 2, \dots \quad (23.67)$$

It is clear from (23.57) that the states in (23.67) are also eigenstates of the oscillator Hamiltonian with the energy eigenvalues

$$E_n = (n + \frac{1}{2})\hbar\omega. \quad (23.68)$$

The states $|n\rangle$, called number states or Fock states, also are eigenstates for the momentum operator of the field mode $\mathbf{q}$ in consideration, viz.

$$\hat{\mathbf{P}} = \hbar \mathbf{q} \hat{N}. \quad (23.69)$$

The eigenvalues of $\hat{\mathbf{P}}$ are given by

$$\mathbf{P}_n = n\hbar \mathbf{q}. \quad (23.70)$$

The eigenvalues of $\hat{H}$ and $\hat{\mathbf{P}}$ are independent of the polarization index s . This is not so for the eigenvalues of the spin operator belonging to a given wave vector $\mathbf{q}$. If we denote the destruction and creation operators for the positive (negative) helicity states by $\hat{a}_+$ ($\hat{a}_-$) and $\hat{a}_+^\dagger$ ($\hat{a}_-^\dagger$), respectively, the number operators for the two species are

$$\hat{N}_\pm = \hat{a}_\pm^\dagger \hat{a}_\pm. \quad (23.71)$$

Since the spin operator is given by (cf. (23.55))

$$\hat{\mathbf{S}} = \hbar \kappa (\hat{N}_+ - \hat{N}_-) \quad (23.72)$$

in the basis of helicity unit vectors, the intrinsic angular momentum of the Fock states $|n_\pm\rangle$, which eigenvalue equations read

$$\hat{N}_\pm |n_\pm\rangle = n_\pm |n_\pm\rangle, \quad n_\pm = 0, 1, 2, \dots, \quad (23.73)$$

are

$$S_{n_\pm} = \pm \hbar \kappa n_\pm. \quad (23.74)$$

Let us now turn our attention towards the eigenstates of the total energy and momentum of the quantized radiation field in the Fock representation. Since the destruction and creation operators of the different $(\mathbf{q}s)$ -modes commute at a fixed time, say $t = 0$ (Schrödinger picture), also the number operators belonging to different modes commute. The eigenstates of $\hat{H}_F$ (23.51) and $\hat{\mathbf{P}}_F$ (23.54), therefore, are the tensor products of the eigenstates of the various $(\mathbf{q}s)$ -modes, i.e.,

$$|n_1, n_2, \dots, n_i, \dots\rangle = |n_1\rangle |n_2\rangle \dots |n_i\rangle \dots, \quad (23.75)$$

where we have used the abbreviated mode notation $i \equiv (\mathbf{q}, s)$. We hence have for the global radiation field

$$\hat{H}_F |n_1, \dots, n_i, \dots\rangle = \left[\sum_i (n_i + \frac{1}{2}) \hbar \omega_i \right] |n_1, \dots, n_i, \dots\rangle, \quad (23.76)$$

and

$$\hat{\mathbf{P}}_F |n_1, \dots, n_i, \dots\rangle = \left[\sum_i n_i \hbar \mathbf{q}_i \right] |n_1, \dots, n_i, \dots\rangle. \quad (23.77)$$

The n_i 's can take on the values $n_i = 0, 1, 2, \dots$. The ground state of the field, which we denote by $|0\rangle$, corresponds to all n_i equal to zero, i.e.,

$$|0\rangle \equiv |0_1, \dots, 0_i, \dots\rangle. \quad (23.78)$$

From (23.67) it is clear that the general eigenstate $|n_1, \dots, n_i, \dots\rangle$ can be obtained from the ground state as follows:

$$|n_1, \dots, n_i, \dots\rangle = \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \dots \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} \dots |0\rangle. \quad (23.79)$$

It appears from the analysis above as if the state $|n_1, \dots, n_i, \dots\rangle$ with respect to the ground state $|0\rangle$ contains n_1 particles with energy $\hbar \omega_1$ and momentum $\hbar \mathbf{q}_1, \dots, n_i$ particles with energy $\hbar \omega_i$ and momentum $\hbar \mathbf{q}_i, \dots$. These particles are called the

monochromatic plane-wave photons, and they describe the elementary excitations of the various modes in the number representation. The photon occupation numbers n_i can assume all values $0, 1, 2, \dots$, and the photons are bosons because the transverse field has been quantized with *commutators*. Particles obeying Fermi–Dirac statistics, such as electrons or muons, come out from a field description where the quantization is with *anticommutators*. For these so-called fermions the occupation numbers in the various modes are restricted to the values 0 and 1. The ground state $|0\rangle$ which has no photons is called the vacuum. According to (23.76) the vacuum has an energy $\sum_i \hbar\omega_i/2$, which is infinite. We shall give some remarks on the physical significance of this later on.

23.2 Temporal Evolution of the Global Field–Matter System

23.2.1 State Space

In order to introduce the general framework for a fully quantized description of the interaction between a system of nonrelativistic charged particles and photons, one must first specify the structure of the state space $\mathcal{E}$ of the total system. First of all, $\mathcal{E}$ is the tensor product of the state spaces of the particles ($\mathcal{E}_P$) and the radiation field ($\mathcal{E}_F$), i.e.,

$$\mathcal{E} = \mathcal{E}_P \otimes \mathcal{E}_F. \quad (23.80)$$

As already mentioned the state space $\mathcal{E}_F$ is itself the product of the state spaces $\mathcal{E}_{F,i}$ of the various oscillators we have associated with the modes of the transverse field:

$$\mathcal{E}_F = \mathcal{E}_{F,1} \otimes \mathcal{E}_{F,2} \otimes \dots \otimes \mathcal{E}_{F,i} \otimes \dots. \quad (23.81)$$

In the state space of the particles the position $\{\hat{\mathbf{r}}_\alpha\}$ and momentum $\{\hat{\mathbf{p}}_\alpha\}$ operators of all particles act. In the state space of the i th field oscillator the annihilation ($\hat{a}_i$) and creation ($\hat{a}_i^\dagger$) operators act. If the set $\{|u\rangle\}$ forms an orthonormal basis of the particle state space, and if we take the set of Fock states $\{|n_i\rangle\}$ as an orthogonal basis of $\mathcal{E}_i$, one can take in the total space $\mathcal{E}$ the following basis

$$\{|u; n_1, n_2, \dots, n_i, \dots\rangle\} = \{|u\rangle|n_1\rangle|n_2\rangle \dots |n_i\rangle \dots\}. \quad (23.82)$$

Other basis choices can be made, of course. With the choice in (23.82) the most general state vector of the particle–photon system is a linear superposition of the basis vectors in the set given in (23.82).

23.2.2 Total Nonrelativistic Hamiltonian in the Coulomb Gauge

If the nonrelativistic particle dynamics is described in the configuration representation, where $\hat{\mathbf{p}}_\alpha = (\hbar/i)\nabla_\alpha$ and $\hat{\mathbf{r}}_\alpha = \mathbf{r}_\alpha$, the total Hamiltonian of the coupled

particle–field system is obtained by adding the Hamilton operator of the transverses field (23.51) to the minimal coupling Hamilton operator (11.101). In the Coulomb gauge, the vector potential appearing in the minimal coupling Hamiltonian is purely transverse [$\mathbf{A} = \mathbf{A}_T$], and in the field-quantized description the operator $\hat{\mathbf{A}}_T$ is given in (23.47). Recalling the analyses in Sects. 9.2.4, 9.3.1 and 9.3.2, we can conclude that the fully quantized Hamilton operator of the coupled particle–field system in the Coulomb gauge is given by the following expression:

$$\hat{H} = \sum_{\alpha} \frac{1}{2m_{\alpha}} \left(\hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}_T(\mathbf{r}_{\alpha}) \right)^2 + \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha} - \mathbf{r}_{\beta}|} + \sum_{\mathbf{q}, s} \hbar \omega_{\mathbf{q}} \left(\hat{a}_{\mathbf{q}s}^{\dagger} \hat{a}_{\mathbf{q}s} + \frac{1}{2} \right), \quad (23.83)$$

leaving out the Coulomb self-energy of the particles.

In the following three subsections, we shall briefly review how the time development of a quantum system can be described in three commonly used pictures, viz., the Schrödinger, Heisenberg and Interaction pictures. Quantities in the three pictures will be distinguished by the labels S, H and I. The labels appear as superscripts on operators, and as subscripts on state vectors. Later on these labels will be omitted whenever it is clear from the context which picture is used.

23.2.3 The Schrödinger Picture

In this picture, the various operators $\hat{\mathcal{O}}^S$ are *essentially* fixed in time. By essential we mean that an *explicit* time dependence *may* occur in $\hat{\mathcal{O}}^S$. As an example of this one has the operator types $\hat{\mathcal{O}}^S(t) = \hat{A}^S f(t)$, where $d\hat{A}^S/dt = 0$. Operators with an explicit time dependence in the Schrödinger picture will not be of significant relevance in this book. The arbitrary state vector $|\psi(t)\rangle_S$ carries all the time evolution of the quantum system in the S-picture according to the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle_S = \hat{H}^S |\psi(t)\rangle_S. \quad (23.84)$$

For the global field–matter Hamiltonian ($\hat{H} = \hat{H}^S$) in (23.83), $|\psi(t)\rangle_S$ can be expanded in the orthonormal basis given in (23.82) for instance, i.e.,

$$|\psi(t)\rangle_S = \sum_{u, n_a, n_2, \dots} C_{un_1 n_2 \dots}(t) |u; n_1, n_2, \dots\rangle. \quad (23.85)$$

If this expansion is inserted into (23.84), the solution of the Schrödinger equation is turned into the solution of a linear system of first-order differential equations among the coefficients $C_{un_1 n_2 \dots}(t)$.

Formally, the solution of the Schrödinger equation in (23.84) can be written as follows:

$$|\psi(t)\rangle_S = \hat{U}(t - t_0) |\psi(t_0)\rangle_S, \quad (23.86)$$

where

$$\hat{U}(\tau) = \exp\left(-\frac{i}{\hbar}\hat{H}^S\tau\right) \quad (23.87)$$

is the so-called (time) evolution operator. A knowledge of the evolution operator allows one to determine the state vector at all times (t) from a given (initial) one at $t = t_0$. The expression for $\hat{U}(\tau)$ in (23.87) presupposes that $\hat{H}^S$ has no explicit time dependence. Since $(\hat{H}^S)^\dagger = \hat{H}^S$, the evolution operator obviously is unitary, i.e.,

$$\hat{U}^{-1}(\tau) = \hat{U}^\dagger(\tau). \quad (23.88)$$

The evolution operator also possesses the properties $\hat{U}^{-1}(\tau) = \hat{U}(-\tau)$, and $\hat{U}(\tau_1 + \tau_2) = \hat{U}(\tau_1)\hat{U}(\tau_2)$.

For the description of many types of field–matter interaction processes it is important to calculate the probability amplitude that a system starting in the initial (i) state $|\psi(t_0)\rangle_S$ at $t = t_0$ ends up in the final (f) state $|\psi(t)\rangle_S$ at $t = t$. The related transition amplitude is just the matrix element of the evolution operator between these states, viz.,

$${}_S\langle\psi_f(t)|\hat{U}(t - t_0)|\psi_i(t_0)\rangle_S. \quad (23.89)$$

23.2.4 The Heisenberg Picture

In this picture the operators $\hat{\mathcal{O}}^H$ evolve in time but the state vector $|\psi\rangle_H$ is fixed. The problem of the temporal evolution of the global system thus is formulated via appropriate equations of motions for the various system variables. One advantage of the Heisenberg point of view is that it is more appropriate for comparisons between the classical and quantum theories than the Schrödinger approach. The state vector in the Heisenberg picture is obtained by operating with $\hat{U}^\dagger(t - t_0)$ on (23.86). Thus, one defines

$$|\psi\rangle_H = \hat{U}^\dagger(t - t_0)\hat{U}(t - t_0)|\psi(t_0)\rangle_S = |\psi(t_0)\rangle_S, \quad (23.90)$$

where the last equality follows from the fact that the evolution operator is unitary (23.88). The fixed Heisenberg state vector thus coincides with the Schrödinger state vector at $t = t_0$. To ensure that physical predictions made in the two pictures at all times will be the same the matrix elements between the arbitrary states A and B must be invariant, i.e.,

$${}_S\langle\psi_B(t)|\hat{\mathcal{O}}^S|\psi_A(t)\rangle_S = {}_H\langle\psi_B|\hat{\mathcal{O}}^H(t)|\psi_A\rangle_H. \quad (23.91)$$

By inserting (23.86) and its associated bra state vector into (23.91), and by remembering (23.90), it appears that operators in the Heisenberg and Schrödinger pictures are related as follows:

$$\hat{O}^H(t) = \hat{U}^\dagger(t - t_0) \hat{O}^S \hat{U}(t - t_0). \quad (23.92)$$

At $t = t_0$, not only the state vectors but also the operators thus are the same in the two pictures. As a consequence of (23.87), the Hamilton operator is time-independent also in the Heisenberg picture that is

$$\hat{H}^H = \hat{H}^S \equiv \hat{H}. \quad (23.93)$$

Differentiation of (23.92) with respect to time gives

$$\frac{d}{dt} \hat{O}^H(t) = \left(\frac{d\hat{U}^\dagger}{dt} \right) \hat{O}^S \hat{U} + \hat{U}^\dagger \hat{O}^S \frac{d\hat{U}}{dt}, \quad (23.94)$$

and from (23.87) one finds

$$\frac{d\hat{U}}{dt} = -\frac{i}{\hbar} \hat{H}^S \hat{U}, \quad (23.95)$$

and thereafter

$$\frac{d\hat{U}^\dagger}{dt} = \frac{i}{\hbar} \hat{U}^\dagger \hat{H}^S, \quad (23.96)$$

since $\hat{H}^S = (\hat{H}^S)^\dagger$. By combining (23.94)–(23.96) one obtains the so-called Heisenberg equation of motion for the operator $\hat{O}^H(t)$, viz.,

$$i\hbar \frac{d}{dt} \hat{O}^H(t) = [\hat{O}^H(t), \hat{H}]. \quad (23.97)$$

The Heisenberg equation in (23.97) plays a central role in the subsequent sections of this chapter. If one allows that the Schrödinger operator $\hat{O}^S$ has an explicit time dependence, the Heisenberg equation of motion is augmented to

$$i\hbar \frac{d}{dt} \hat{O}^H(t) = [\hat{O}^H(t), \hat{H}] + i\hbar \left(\frac{\partial \hat{O}^S}{\partial t} \right)^H, \quad (23.98)$$

where the last term is the Heisenberg representative of the Schrödinger operator $\partial \hat{O}^S / \partial t$, multiplied by $i\hbar$.

23.2.5 The Interaction Picture

It is often useful to divide the global Hamiltonian into two parts

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \quad (23.99)$$

where typically $\hat{H}_I$ is a Hamilton operator describing the interaction (subscript I) between two subsystems which themselves are described by the Hamiltonian $\hat{H}_0$ in the absence of interaction. The Interaction picture is related to the Schrödinger picture by the unitary transformation

$$\hat{U}_0(\tau) = \exp\left(-\frac{i}{\hbar} \hat{H}_0 \tau\right), \quad (23.100)$$

i.e.,

$$|\psi(t)\rangle_I = \hat{U}_0^\dagger(t - t_0) |\psi(t)\rangle_S, \quad (23.101)$$

and

$$\hat{\mathcal{O}}^I(t) = \hat{U}_0^\dagger(t - t_0) \hat{\mathcal{O}}^S \hat{U}_0(t - t_0). \quad (23.102)$$

The last equation ensures that matrix elements between arbitrary states are invariant. From (23.102) one obtains

$$\hat{H}_0^I = \hat{H}_0^S \equiv \hat{H}_0, \quad (23.103)$$

and also

$$i\hbar \frac{d}{dt} \hat{\mathcal{O}}^I(t) = [\hat{\mathcal{O}}^I(t), \hat{H}_0], \quad (23.104)$$

as the reader may verify to himself. With the help of the Schrödinger equation in (23.84), it is not difficult to show that the state vector in the Interaction picture obeys the dynamical equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle_I = \hat{H}_I^I(t) |\psi(t)\rangle_I, \quad (23.105)$$

where

$$\hat{H}_I^I(t) = \exp\left[\frac{i}{\hbar} \hat{H}_0(t - t_0)\right] \hat{H}_I^S \exp\left[-\frac{i}{\hbar} \hat{H}_0(t - t_0)\right] \quad (23.106)$$

is the interaction operator in the interaction picture. In this picture, both operators and state vectors depend on time, in general.

23.3 The Quantized Newton–Lorentz Equation

Let us now apply the Heisenberg equation of motion in (23.97) to two different operators belonging to particle number α , viz., the position operator $\hat{\mathbf{r}}_\alpha$ and the mechanical (kinematical) momentum operator

$$\hat{\boldsymbol{\pi}}_\alpha = \hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\hat{\mathbf{r}}_\alpha). \quad (23.107)$$

For the following calculations, it will be useful to evaluate certain commutators involving $\hat{\mathbf{r}}_\alpha$ and $\hat{\boldsymbol{\pi}}_\alpha$. Starting from the fundamental commutator

$$[\hat{r}_{\alpha,i}, \hat{\pi}_{\alpha,j}] = [\hat{r}_{\alpha,i}, \hat{p}_{\alpha,j}] = i\hbar\delta_{ij}, \quad (23.108)$$

one obtains

$$\begin{aligned} [\hat{r}_{\alpha,i}, \hat{\pi}_{\alpha,j}^2] &= [\hat{r}_{\alpha,i}, \hat{\pi}_{\alpha,j}] \hat{\pi}_{\alpha,j} + \hat{\pi}_{\alpha,j} [\hat{r}_{\alpha,i}, \hat{\pi}_{\alpha,j}] \\ &= 2i\hbar\delta_{ij} \hat{\pi}_{\alpha,j}, \end{aligned} \quad (23.109)$$

and

$$\begin{aligned} [\hat{\pi}_{\alpha,i}, \hat{\pi}_{\alpha,j}] &= -q_\alpha \left\{ [\hat{p}_{\alpha,i}, \hat{A}_{T,j}(\hat{\mathbf{r}}_\alpha)] + [\hat{A}_{T,i}(\hat{\mathbf{r}}_\alpha), \hat{p}_{\alpha,j}] \right\} \\ &= i\hbar q_\alpha \left[\frac{\partial}{\partial \hat{r}_{\alpha,i}} \hat{A}_{T,j}(\hat{\mathbf{r}}_\alpha) - \frac{\partial}{\partial \hat{r}_{\alpha,j}} \hat{A}_{T,i}(\hat{\mathbf{r}}_\alpha) \right] \\ &= i\hbar q_\alpha \sum_k \epsilon_{ijk} \hat{B}_k(\hat{\mathbf{r}}_\alpha). \end{aligned} \quad (23.110)$$

In order to determine the Heisenberg equation for the particle position operator, one notes that $\hat{\mathbf{r}}_\alpha$ commutes with all the operators in $\hat{H}$, except $\hat{\mathbf{p}}_\alpha$. Therefore,

$$\frac{d}{dt} \hat{\mathbf{r}}_\alpha = (i\hbar)^{-1} [\hat{\mathbf{r}}_\alpha, \hat{H}] = (2i\hbar m_\alpha)^{-1} [\hat{\mathbf{r}}_\alpha, \hat{\boldsymbol{\pi}}_\alpha \cdot \hat{\boldsymbol{\pi}}_\alpha], \quad (23.111)$$

and then by means of (23.109)

$$m_\alpha \hat{\mathbf{v}}_\alpha = \hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\hat{\mathbf{r}}_\alpha), \quad (23.112)$$

where $\hat{\mathbf{v}}_\alpha = d\hat{\mathbf{r}}_\alpha/dt$ is the velocity operator of the particle. Equation (23.112) thus is just the operator version of the well known nonrelativistic relation between the mechanical ($m_\alpha \mathbf{v}_\alpha$) and canonical ($\mathbf{p}_\alpha$) momenta, see (9.82).

The Heisenberg equation for the mechanical momentum operator

$$\frac{d}{dt} \hat{\boldsymbol{\pi}}_\alpha = (i\hbar)^{-1} [\hat{\boldsymbol{\pi}}_\alpha, \hat{H}] \quad (23.113)$$

leads to the quantum form of the Newton–Lorentz equation, as we soon shall see. To trace the origin of the various parts of the quantum Lorentz force, we consider the commutator of $\hat{\boldsymbol{\pi}}_\alpha$ with each of the three (double) sums in (23.83). The commutator with the radiation-field Hamiltonian

$$(i\hbar)^{-1} \left[\hat{\boldsymbol{\pi}}_\alpha, \sum_{\mathbf{q},s} \hbar\omega_{\mathbf{q}} \left(\hat{a}_{\mathbf{q}s}^\dagger \hat{a}_{\mathbf{q}s} + \frac{1}{2} \right) \right] = i q_\alpha \sum_{\mathbf{q},s} [\hat{\mathbf{A}}_T(\hat{\mathbf{r}}_\alpha), \omega_{\mathbf{q}} \hat{a}_{\mathbf{q}s}^\dagger \hat{a}_{\mathbf{q}s}], \quad (23.114)$$

is calculated with the help of (23.47), evaluated for $\hat{\mathbf{r}} = \hat{\mathbf{r}}_\alpha$. The expression for $\hat{\mathbf{A}}_T(\hat{\mathbf{r}}_\alpha)$ contains a summation over modes ($\mathbf{q}, s$). On top of this we have a summation over modes (running indices ($\mathbf{q}', s'$), say) in (23.114). Thanks to (23.45)

and (23.46), we only obtain contributions for mode combinations where $(\mathbf{q}, s) = (\mathbf{q}', s')$. In these combinations appear the commutators

$$[\hat{a}_{qs}, \hat{N}_{qs}] = \hat{a}_{qs}, \quad (23.115)$$

$$[\hat{a}_{qs}^\dagger, \hat{N}_{qs}] = -\hat{a}_{qs}^\dagger. \quad (23.116)$$

The opposite signs on the right sides of these equations, and the factor $i\omega_q$ finally gives

$$iq_\alpha \sum_{\mathbf{q}, s} [\hat{A}_T(\hat{\mathbf{r}}_\alpha), \omega_q \hat{N}_{qs}] = q_\alpha \hat{\mathbf{E}}_T(\hat{\mathbf{r}}_\alpha), \quad (23.117)$$

where the transverse electric field operator has the mode expansion in (23.49). The commutator between $\hat{\boldsymbol{\pi}}_\alpha$ and the Coulomb part of the Hamiltonian in (23.83) is readily obtained. Thus,

$$\begin{aligned} (i\hbar)^{-1} [\hat{\boldsymbol{\pi}}_\alpha, V_{\text{coul}}] &= (i\hbar)^{-1} [\hat{\mathbf{p}}, V_{\text{coul}}] \\ &= -\nabla_\alpha V_{\text{coul}} = q_\alpha \hat{\mathbf{E}}_L(\hat{\mathbf{r}}_\alpha). \end{aligned} \quad (23.118)$$

Together, the contribution to the right-hand-side of (23.113) from the radiation and Coulomb parts of the global Hamiltonian hence give $q_\alpha(\hat{\mathbf{E}}_T(\hat{\mathbf{r}}_\alpha) + \hat{\mathbf{E}}_L(\hat{\mathbf{r}}_\alpha)) = q_\alpha \hat{\mathbf{E}}(\hat{\mathbf{r}}_\alpha)$, i.e., an operator version of the electric field part of the Lorentz force. The commutator between $\hat{\boldsymbol{\pi}}_\alpha$ and the kinetic energy part of $\hat{H}$, essentially

$$(i\hbar)^{-1} \left[\hat{\boldsymbol{\pi}}_\alpha, \sum_\beta \frac{1}{2m_\beta} \hat{\boldsymbol{\pi}}_\beta \cdot \hat{\boldsymbol{\pi}}_\beta \right] = (2i\hbar m_\alpha)^{-1} [\hat{\boldsymbol{\pi}}_\alpha, \hat{\boldsymbol{\pi}}_\alpha \cdot \hat{\boldsymbol{\pi}}_\alpha], \quad (23.119)$$

can be evaluated using the result in (23.110). For the i th component we obtain

$$\begin{aligned} &(2i\hbar m_\alpha)^{-1} \sum_j [\hat{\pi}_{\alpha,i}, \hat{\pi}_{q,j}^2] \\ &= (2i\hbar m_\alpha)^{-1} \sum_j \{ \hat{\pi}_{\alpha,j} [\hat{\pi}_{\alpha,i}, \hat{\pi}_{\alpha,j}] + [\hat{\pi}_{\alpha,i}, \hat{\pi}_{\alpha,j}] \hat{\pi}_{\alpha,j} \} \\ &= \frac{q_\alpha}{2m_\alpha} \sum_{j,k} \epsilon_{ijk} (\hat{\pi}_{\alpha,j} \hat{B}_k + \hat{B}_k \hat{\pi}_{\alpha,j}). \end{aligned} \quad (23.120)$$

It is not difficult to demonstrate that the last expression in this equation is just the i th component of the vector

$$\frac{q_\alpha}{2} (\hat{\mathbf{v}}_\alpha \times \hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha) - \hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha) \times \hat{\mathbf{v}}_\alpha). \quad (23.121)$$

This vector can be considered as the magnetic part of a symmetrized Lorentz force operator. The symmetrization ensures that the operator is Hermitian. By regrouping the preceding results we finally have

$$m_\alpha \frac{d^2}{dt^2} \hat{\mathbf{r}}_\alpha = q_\alpha \left\{ \hat{\mathbf{E}}(\hat{\mathbf{r}}_\alpha) + \frac{1}{2} \left[\hat{\mathbf{v}}_\alpha \times \hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha) - \hat{\mathbf{B}}(\hat{\mathbf{r}}_\alpha) \times \hat{\mathbf{v}}_\alpha \right] \right\}. \quad (23.122)$$

The operator equation in (23.122) is the quantum form of the nonrelativistic Newton–Lorentz equation.

23.4 The Quantized Maxwell–Lorentz Equations in the Coulomb Gauge

23.4.1 Equation of Motion for the Annihilation Operator, $\hat{a}_{qs}$

The Heisenberg equation,

$$i\hbar \frac{d}{dt} \hat{a}_{qs}(t) = [\hat{a}_{qs}(t), \hat{H}], \quad (23.123)$$

allows us to determine the time evolution of the annihilation operator of the mode (qs). The Coulomb energy in (23.83) does not contribute to the commutator in (23.123), and the contribution from the radiation field is readily determined with the help of the fundamental commutator relations in (23.45) and (23.46). Thus,

$$\begin{aligned} \left[\hat{a}_{qs}, \sum_{q',s'} \hbar\omega_{q'} \left(\hat{a}_{q's'}^\dagger \hat{a}_{q's'} + \frac{1}{2} \right) \right] &= \hbar\omega_q [\hat{a}_{qs}, \hat{a}_{qs}^\dagger \hat{a}_{qs}] \\ &= \hbar\omega_q \left[(\hat{a}_{qs}^\dagger \hat{a}_{qs} + 1) \hat{a}_{qs} - \hat{a}_{qs}^\dagger \hat{a}_{qs} \hat{a}_{qs} \right] \\ &= \hbar\omega_q \hat{a}_{qs}. \end{aligned} \quad (23.124)$$

The reduction of the commutator part containing the kinetic energy operator of the particles requires a bit of algebra. To carry out the calculation it is useful to begin from a quite general result, viz.,

$$[\hat{a}, (\hat{a}^\dagger)^n] = n(\hat{a}^\dagger)^{n-1}, \quad n = 1, 2, \dots. \quad (23.125)$$

The correctness of this relation may be proved by induction. Equation (23.125) certainly is correct for $n = 1$ (23.46). By assuming that the result holds for $n = n$, it is easy to show that it holds also for $n = n + 1$. Thus,

$$\begin{aligned}
\left[\hat{a}, (\hat{a}^\dagger)^{n+1} \right] &= \hat{a}(\hat{a}^\dagger)^n \hat{a}^\dagger - (\hat{a}^\dagger)^n \hat{a}^\dagger \hat{a} \\
&= \left((\hat{a}^\dagger)^n \hat{a} + n(\hat{a}^\dagger)^{n-1} \right) \hat{a}^\dagger - (\hat{a}^\dagger)^n \hat{a}^\dagger \hat{a} \\
&= (\hat{a}^\dagger)^n \left(\hat{a} \hat{a}^\dagger - \hat{a}^\dagger \hat{a} \right) + n(\hat{a}^\dagger)^n \\
&= (n+1)(\hat{a}^\dagger)^n,
\end{aligned} \tag{23.126}$$

as we wanted to prove. The relation in (23.125) can be used to derive a simple result for the commutator between $\hat{a}$ and a function $f(\hat{a}, \hat{a}^\dagger)$ which can be expressed in a power series in $\hat{a}^\dagger$ that is

$$f(\hat{a}, \hat{a}^\dagger) = \sum_{n=0}^{\infty} \alpha_n(\hat{a}) (\hat{a}^\dagger)^n. \tag{23.127}$$

Hence,

$$\begin{aligned}
\left[\hat{a}, f(\hat{a}, \hat{a}^\dagger) \right] &= \sum_{n=0}^{\infty} \alpha_n(\hat{a}) \left[\hat{a}, (\hat{a}^\dagger)^n \right] \\
&= \sum_{n=1}^{\infty} \alpha_n(\hat{a}) n (\hat{a}^\dagger)^{n-1} \\
&= \frac{\partial}{\partial \hat{a}^\dagger} f(\hat{a}, \hat{a}^\dagger).
\end{aligned} \tag{23.128}$$

By utilizing (23.128), one obtains [$i \equiv (\mathbf{q}s)$]

$$\left[\hat{a}_i, \sum_{\alpha} \frac{m_{\alpha}}{2} \hat{\mathbf{v}}_{\alpha} \cdot \hat{\mathbf{v}}_{\alpha} \right] = \sum_{\alpha} \frac{m_{\alpha}}{2} \left[\left(\frac{\partial}{\partial \hat{a}_i^\dagger} \hat{\mathbf{v}}_{\alpha} \right) \cdot \hat{\mathbf{v}}_{\alpha} + \mathbf{v}_{\alpha} \cdot \frac{\partial}{\partial \hat{a}_i^\dagger} \hat{\mathbf{v}}_{\alpha} \right]. \tag{23.129}$$

With the expansion for $\hat{\mathbf{A}}_{\text{T}}(\hat{\mathbf{r}}_{\alpha})$ (23.47) inserted into (23.112) it is easy to show that

$$\frac{\partial}{\partial \hat{a}_i^\dagger} \hat{\mathbf{v}}_{\alpha} = -\frac{q_{\alpha}}{m_{\alpha}} \left(\frac{\hbar}{2\epsilon_0 \omega_i L^3} \right)^{1/2} \boldsymbol{\epsilon}_i e^{-i\mathbf{q}_i \cdot \hat{\mathbf{r}}_{\alpha}}, \tag{23.130}$$

and this then gives

$$\left[\hat{a}_i, \sum_{\alpha} \frac{m_{\alpha}}{2} \hat{\mathbf{v}}_{\alpha} \cdot \hat{\mathbf{v}}_{\alpha} \right] = -\left(\frac{\hbar}{2\epsilon_0 \omega_i L^3} \right)^{1/2} \boldsymbol{\epsilon}_i \cdot \left[\sum_{\alpha} \frac{q_{\alpha}}{2} \left(\hat{\mathbf{v}}_{\alpha} e^{-i\mathbf{q}_i \cdot \hat{\mathbf{r}}_{\alpha}} + e^{-i\mathbf{q}_i \cdot \hat{\mathbf{r}}_{\alpha}} \mathbf{v}_{\alpha} \right) \right]. \tag{23.131}$$

The result in (23.131) can be expressed in an appealing manner if one introduces the symmetric current density operator ($\hat{\mathbf{j}}(\mathbf{r}) \equiv \hat{\mathbf{J}}(\mathbf{r})$ in what follows)

$$\hat{\mathbf{J}}(\mathbf{r}) = \frac{1}{2} \sum_{\alpha} q_{\alpha} [\hat{\mathbf{v}}_{\alpha} \delta(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}) + \delta(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}) \hat{\mathbf{v}}_{\alpha}]. \quad (23.132)$$

The symmetrization procedure makes the operator Hermitian, i.e.,

$$\hat{\mathbf{J}}(\mathbf{r}) = \hat{\mathbf{J}}^{\dagger}(\mathbf{r}). \quad (23.133)$$

The spatial Fourier transform of $\hat{\mathbf{J}}(\mathbf{r})$, namely

$$\hat{\mathbf{J}}(\mathbf{q}) = L^{-3/2} \int_V \hat{\mathbf{J}}(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} d^3r, \quad (23.134)$$

is given by

$$\hat{\mathbf{J}}(\mathbf{q}) = L^{-3/2} \sum_{\alpha} \frac{q_{\alpha}}{2} \left(\hat{\mathbf{v}}_{\alpha} e^{-i\mathbf{q} \cdot \hat{\mathbf{r}}_{\alpha}} + e^{-i\mathbf{q} \cdot \hat{\mathbf{r}}_{\alpha}} \hat{\mathbf{v}}_{\alpha} \right), \quad (23.135)$$

and it is precisely this quantity taken for $\mathbf{q} = \mathbf{q}_i$ which enters (23.131). With the replacement $i \Rightarrow (\mathbf{q}, s)$, (23.131) finally takes the form

$$\left[\hat{a}_{qs}, \sum_{\alpha} \frac{m_{\alpha}}{2} \hat{\mathbf{v}}_{\alpha} \cdot \hat{\mathbf{v}}_{\alpha} \right] = - \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{J}}(\mathbf{q}). \quad (23.136)$$

If one gathers the results in (23.124) and (23.136) it follows that the dynamical equation for the annihilation operator $\hat{a}_{qs}$ is

$$\frac{d}{dt} \hat{a}_{qs} = -i\omega_q \hat{a}_{qs} + i(2\epsilon_0 \hbar \omega_q)^{-1/2} \boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{J}}(\mathbf{q}). \quad (23.137)$$

The equation of motion for the creation operator $\hat{a}_{qs}^{\dagger}$ is obtained by Hermitian conjugation of (23.137). Hence,

$$\frac{d}{dt} \hat{a}_{qs}^{\dagger} = i\omega_q \hat{a}_{qs}^{\dagger} - i(2\epsilon_0 \hbar \omega_q)^{-1/2} \boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{J}}(-\mathbf{q}), \quad (23.138)$$

since $\hat{\mathbf{J}}^{\dagger}(\mathbf{q}) = \hat{\mathbf{J}}(-\mathbf{q})$, remembering that $\hat{\mathbf{v}}_{\alpha}^{\dagger} = \hat{\mathbf{v}}_{\alpha}$.

In the absence of particles ($\hat{\mathbf{J}}(\mathbf{q}) = \mathbf{0}$), the solutions to (23.137) and (23.138) are precisely those already given in (23.43) and (23.44). In the Heisenberg picture the operators associated with the free fields $\hat{\mathbf{A}}_T$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{E}}_T$ are obtained by inserting (23.43) and (23.44) into the expansions given in (23.47)–(23.49). For example, one obtains for the transverse vector-potential operator

$$\hat{\mathbf{A}}_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \left[\hat{a}_{qs}(0) e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_q t)} + h.c. \right] \boldsymbol{\epsilon}_{qs}. \quad (23.139)$$

The expansion thus is in linearly polarized plane waves, and the time-independent coefficients (operators) $\hat{a}_{qs}(0)$ and $\hat{a}_{qs}^\dagger(0)$ satisfy the commutation relations in (23.41) and (23.42).

23.4.2 Equations of Motions for the Transverse Electric ($\hat{\mathbf{E}}_T$) and Magnetic ($\hat{\mathbf{B}}$) Field Operators

The dynamical equations of motions for $\hat{a}_{qs}$ and $\hat{a}_{qs}^\dagger$ are very helpful in the analyses of the time development of the transverse electric and magnetic field operators. In the Heisenberg picture, the time derivative of $\hat{\mathbf{E}}_T(\mathbf{r})$ is given by

$$c_0^{-2} \frac{\partial}{\partial t} \hat{\mathbf{E}}_T(\mathbf{r}, t) = c_0^{-2} L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0} \right)^{1/2} \times \left[\left(\frac{d}{dt} \hat{a}_{qs} \right) e^{i\mathbf{q} \cdot \mathbf{r}} - \left(\frac{d}{dt} \hat{a}_{qs}^\dagger \right) e^{-i\mathbf{q} \cdot \mathbf{r}} \right] \boldsymbol{\epsilon}_{qs}, \quad (23.140)$$

cf. (23.49). When (23.137) and (23.138) are inserted into this equation, one obtains

$$c_0^{-2} \frac{\partial}{\partial t} \hat{\mathbf{E}}_T(\mathbf{r}, t) = \hat{\mathcal{O}}_1(\mathbf{r}, t) + \hat{\mathcal{O}}_2(\mathbf{r}, t), \quad (23.141)$$

where $\hat{\mathcal{O}}_1(\mathbf{r}, t)$ is the part associated with the homogeneous terms, $-i\omega\hat{a}_{qs}$ ($i\omega\hat{a}_{qs}^\dagger$), and $\hat{\mathcal{O}}_2(\mathbf{r}, t)$ is the part containing the current density operator $\hat{\mathbf{J}}(\mathbf{q})$ and its Hermitian conjugate. A simple calculation shows that

$$\begin{aligned} \hat{\mathcal{O}}_1(\mathbf{r}, t) &= L^{-3/2} \sum_{q,s} \left(\frac{\hbar \omega_q}{2\epsilon_0 c_0^2} \right)^{1/2} \frac{\omega_q}{c_0} \left(\hat{a}_{qs}(t) e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{a}_{qs}^\dagger(t) e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \boldsymbol{\epsilon}_{qs} \\ &= \nabla \times \hat{\mathbf{B}}(\mathbf{r}, t), \end{aligned} \quad (23.142)$$

where $\hat{\mathbf{B}}(\mathbf{r}, t)$ is the Heisenberg representative of (23.48). The second part is given by

$$\hat{\mathcal{O}}_2(\mathbf{r}, t) = -\mu_0 L^{-3/2} \sum_{q,s} \frac{1}{2} \left(\hat{\mathbf{J}}(\mathbf{q}; t) e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{\mathbf{J}}(-\mathbf{q}; t) e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \cdot \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs}. \quad (23.143)$$

By utilizing (15.52), and making the variable change $\mathbf{q} \Rightarrow -\mathbf{q}$ in the last summation over $\mathbf{q}$, (23.143) can be reduced to the shorter form

$$\hat{\mathcal{O}}_2(\mathbf{r}, t) = -\mu_0 L^{-3/2} \sum_{\mathbf{q}} \hat{\mathbf{J}}(\mathbf{q}; t) e^{i\mathbf{q} \cdot \mathbf{r}} \cdot (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}). \quad (23.144)$$

The expression for $\hat{\mathcal{O}}_2(\mathbf{r}, t)$ can be rewritten in a physically appealing form as we shall see now. Thus, we first insert the expression given in (23.135) for $\hat{\mathbf{J}}(\mathbf{q}; t)$ into (23.144). Upon interchange of the α - and $\mathbf{q}$ -summations we obtain

$$\hat{\mathcal{O}}_2(\mathbf{r}, t) = -\mu_0 \sum_{\alpha} \frac{q_{\alpha}}{2} \left\{ L^{-3} \sum_{\mathbf{q}} \left[\hat{\mathbf{v}}_{\alpha} e^{i\mathbf{q} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha})} + e^{i\mathbf{q} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha})} \hat{\mathbf{v}}_{\alpha} \right] \cdot (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}) \right\}. \quad (23.145)$$

Next, we take the limit $L \rightarrow \infty$. This gives according to the rule in (23.1)

$$\hat{\mathcal{O}}_2(\mathbf{r}, t) = -\mu_0 \sum_{\alpha} \frac{q_{\alpha}}{2} \int_{-\infty}^{\infty} \left[\hat{\mathbf{v}}_{\alpha} e^{i\mathbf{q} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha})} + e^{i\mathbf{q} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha})} \hat{\mathbf{v}}_{\alpha} \right] \cdot (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}) \frac{d^3 q}{(2\pi)^3}. \quad (23.146)$$

With the help of the transverse delta function operator

$$\delta_{\text{T}}(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}) = \int_{-\infty}^{\infty} (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}) e^{i\mathbf{q} \cdot (\mathbf{r} - \hat{\mathbf{r}}_{\alpha})} \frac{d^3 q}{(2\pi)^3}, \quad (23.147)$$

we finally get

$$\hat{\mathcal{O}}_2(\mathbf{r}, t) = -\mu_0 \hat{\mathbf{J}}_{\text{T}}(\mathbf{r}, t), \quad (23.148)$$

where

$$\hat{\mathbf{J}}_{\text{T}}(\mathbf{r}, t) = \frac{1}{2} \sum_{\alpha} q_{\alpha} [\hat{\mathbf{v}}_{\alpha} \cdot \delta_{\text{T}}(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}) + \delta_{\text{T}}(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}) \cdot \hat{\mathbf{v}}_{\alpha}]. \quad (23.149)$$

A comparison of (23.132) and (23.149) shows that $\hat{\mathbf{J}}_{\text{T}}(\mathbf{r}, t)$ is the transverse part of the symmetrized (Hermitian) current density operator $\hat{\mathbf{J}}(\mathbf{r}, t)$. By gathering (23.141), (23.142) and (23.148), we obtain the dynamical equation

$$\nabla \times \hat{\mathbf{B}}(\mathbf{r}, t) = \mu_0 \hat{\mathbf{J}}_{\text{T}}(\mathbf{r}, t) + c_0^{-2} \frac{\partial}{\partial t} \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t). \quad (23.150)$$

This result is just the Heisenberg operator version of the transverse Maxwell–Lorentz equation in (9.26).

Let us now turn the attention towards the time derivative of the magnetic field operator in the Heisenberg picture. By differentiation of (23.48) with respect to time and afterwards use of (23.137) and (23.138), we again obtain two parts

$$\frac{\partial}{\partial t} \hat{\mathbf{B}}(\mathbf{r}, t) = \hat{\mathcal{P}}_1(\mathbf{r}, t) + \hat{\mathcal{P}}_2(\mathbf{r}, t). \quad (23.151)$$

It is easy to demonstrate that the part $\hat{\mathcal{P}}_1(\mathbf{r}, t)$, which is associated to the homogeneous terms in the dynamical equations for the annihilation and creation operators, is given by

$$\hat{\mathcal{P}}_1(\mathbf{r}, t) = -\nabla \times \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t). \quad (23.152)$$

The other part becomes

$$\begin{aligned}\hat{\mathcal{P}}_2(\mathbf{r}, t) &= L^{-3/2}(2\epsilon_0 c_0)^{-1} \sum_{\mathbf{q}, s} \left(\hat{\mathbf{J}}(\mathbf{q}; t) e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{\mathbf{J}}(-\mathbf{q}; t) e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \cdot \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} \times \boldsymbol{\kappa} \\ &= L^{-3/2}(2\epsilon_0 c_0)^{-1} \sum_{\mathbf{q}} \left(\hat{\mathbf{J}}(\mathbf{q}; t) e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{\mathbf{J}}(-\mathbf{q}; t) e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \times \boldsymbol{\kappa}.\end{aligned}\quad (23.153)$$

By making the substitution $\mathbf{q} \Rightarrow -\mathbf{q}$ (and thus $\boldsymbol{\kappa} \Rightarrow -\boldsymbol{\kappa}$) in the last sum, one immediately obtains

$$\hat{\mathcal{P}}_2(\mathbf{r}, t) = \mathbf{0}. \quad (23.154)$$

Together, (23.151), (23.152), and (23.154) hence lead to the Heisenberg operator version,

$$\nabla \times \hat{\mathbf{E}}_T(\mathbf{r}, t) = -\frac{\partial}{\partial t} \hat{\mathbf{B}}(\mathbf{r}, t), \quad (23.155)$$

of the transverse Maxwell–Lorentz equation in (9.25). The Maxwell operator equation $\nabla \cdot \hat{\mathbf{B}}(\mathbf{r}, t) = 0$, which express the transversality of $\hat{\mathbf{B}}(\mathbf{r}, t)$ follows directly from the Heisenberg version of (23.48).

23.4.3 Longitudinal Electric Field Operator

This operator only depends on the position operators of the various particles, and its explicit form is given by

$$\hat{\mathbf{E}}_L(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{\alpha} \frac{q_{\alpha}(\mathbf{r} - \hat{\mathbf{r}}_{\alpha})}{|\mathbf{r} - \hat{\mathbf{r}}_{\alpha}|^3}, \quad (23.156)$$

as one realizes by a translation of (9.54) to operator form. In the Heisenberg picture the time dependence of $\hat{\mathbf{E}}_L$ appears through the time dependence of the $\hat{\mathbf{r}}_{\alpha}$ -operators, cf. (23.111) and (23.112). The longitudinal electric field operator satisfies in the Heisenberg picture the operator version

$$\nabla \cdot \hat{\mathbf{E}}_L(\mathbf{r}, t) = \frac{1}{\epsilon_0} \hat{\rho}(\mathbf{r}, t) \quad (23.157)$$

of the Maxwell equation in (9.27). In (23.157), $\hat{\rho}$ is the charge density operator, i.e.,

$$\hat{\rho}(\mathbf{r}, t) = \sum_{\alpha} q_{\alpha} \delta(\mathbf{r} - \hat{\mathbf{r}}_{\alpha}(t)). \quad (23.158)$$

The classical relation in (9.27) can of course also be extended to the operator level if needed. When combined, the operator versions of (9.27) and (23.157) lead to the charge equation of continuity on operator form.

Chapter 24

Field Commutators and Integral Representation of Various Covariant Propagators

It is important to study the commutator relations between different field operators (observables) because these provide us with information on the compatibility of the measurements of two field quantities in space–time [178, 316, 317, 356–359]. We begin our investigation with calculations of free-field commutators taken at different space–time points, and we focus our attention on the commutators among $\hat{\mathbf{E}}_T$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{A}}_T$. It is shown that all commutators involving the transverse electric and magnetic fields are zero outside the forward and backward light cones. For near-field quantum electrodynamics the commutator $[\hat{\mathbf{A}}_T(\mathbf{r}, t), \hat{\mathbf{E}}_T(\mathbf{r}', t')]$ turns out to be of particular importance because it contains a rim zone part which is nonvanishing for space-like separations of the two space–time points in consideration.

The equal-time commutators $[\hat{\mathbf{E}}_T(\mathbf{r}, t), \hat{\mathbf{E}}_T(\mathbf{r}', t)] = c_0^2[\hat{\mathbf{B}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t)]$ vanish for all combinations of $\mathbf{r}$ and $\mathbf{r}'$, whereas $[\hat{\mathbf{E}}_T(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t)]$ is different from zero if $\mathbf{r} = \mathbf{r}'$, and proportional to the dyad $\mathbf{U} \times \nabla \delta(\mathbf{r} - \mathbf{r}')$. Components of the transverse electric and magnetic fields along the same axis therefore always commute. The equal-time commutator $[\hat{\mathbf{A}}_T(\mathbf{r}, t), \hat{\mathbf{E}}_T(\mathbf{r}', t)]$ turns out to be proportional to the transverse delta function, $\delta_T(\mathbf{r} - \mathbf{r}')$, which is nonvanishing if the two points are located in each others rim zones. In the presence of field–matter interaction, there are no simple expressions for the various field commutators, unless these are evaluated at equal times.

The field commutators in general involve singular functions (delta functions and their first and second derivatives). This singular behavior does not harm the physics, because field measurements only can be carried out over space–time regions of finite size [178, 316, 317]. We briefly discuss weighted space-averaging of fields and commutators.

In the studies of the field commutators the so-called Jordan–Pauli scalar propagator plays an important role [358], and therefore we analyze this propagator, as well as its real and imaginary parts. From the Jordan–Pauli propagator one is readily led to another important scalar propagator, the Feynman propagator, also named the meson propagator [155]. From the Feynman scalar propagator the route to the covariant photon propagator is short, and this propagator has a prominent position in the covariant theory of near-field quantum electrodynamics. We finish this chapter with a brief introduction to the contour integral representations of the Jordan–Pauli and Feynman propagators.

24.1 The Jordan–Pauli and Feynman Scalar Propagators

It is useful for the subsequent studies of the various field commutators, the dynamical time evolution of the field operators, and the covariant photon propagator to introduce the function

$$\Delta^+(x) \equiv \frac{c_0^2}{2i} \int_{-\infty}^{\infty} e^{-iq_\mu x^\mu} \frac{d^3 q}{(2\pi)^3 \omega_q}, \quad (24.1)$$

where

$$\omega_q = c_0[q^2 + (\frac{mc_0}{\hbar})^2]^{1/2}. \quad (24.2)$$

Equation (24.2) is the relativistic dispersion relation for a particle with rest mass m . For brevity, the covariant notation $[x = \{x^\mu\} = (c_0\tau, \mathbf{R})$ and $-q_\mu x^\mu = \mathbf{q} \cdot \mathbf{R} - \omega_q \tau$] has been used. Two important propagators emerge by combination of $\Delta^+(x)$ and its complex conjugate

$$\Delta^-(x) \equiv (\Delta^+(x))^* = -\frac{c_0^2}{2i} \int_{-\infty}^{\infty} e^{iq_\mu x^\mu} \frac{d^3 q}{(2\pi)^3 \omega_q}. \quad (24.3)$$

The one is the massive Feynman (subscript F) scalar propagator

$$\Delta_F(x) \equiv \theta(\tau)\Delta^+(x) - \theta(-\tau)\Delta^-(x), \quad (24.4)$$

$\theta(\tau)$ being the Heaviside step function, and the other,

$$\Delta_{JP}(x) \equiv \Delta^+(x) + \Delta^-(x), \quad (24.5)$$

is the real massive Jordan–Pauli (JP) scalar propagator. The functions Δ^- , Δ^+ , Δ_F and Δ_{JP} all satisfy the Klein–Gordon equation. If spherical coordinates are used in (24.1), it is easy to carry out the integrations over the polar and azimuth angles. Doing this, one obtains the following one-dimensional integral representation of $\Delta^+(x)$:

$$\Delta^+(R, \tau) = -\frac{c_0^2}{8\pi^2 R} \int_0^\infty \frac{q}{\omega_q} \left[e^{i(qR - \omega_q \tau)} - e^{-i(qR + \omega_q \tau)} \right] dq. \quad (24.6)$$

For a massless particle [$\omega_q = c_0 q$], (24.6) is reduced to

$$\begin{aligned} \Delta^+(R, \tau) &= -\frac{c_0}{8\pi^2 R} \int_0^\infty \left[e^{iq(R - c_0 \tau)} - e^{-iq(R + c_0 \tau)} \right] dq \\ &= -\frac{c_0}{4\pi R} \left[\delta^{(+)}(R - c_0 \tau) - \delta^{(-)}(R + c_0 \tau) \right], \end{aligned} \quad (24.7)$$

where, in the last expression, we have introduced the positive- and negative-wave-number parts of the Dirac delta functions $\delta(R \mp c_0\tau)$. On the basis of (15.42), it appears that the real and imaginary parts of $\Delta^+(R, \tau)$ are given by

$$\Re \Delta^+(R, \tau) = \frac{1}{8\pi R} \left[\delta\left(\frac{R}{c_0} + \tau\right) - \delta\left(\frac{R}{c_0} - \tau\right) \right], \quad (24.8)$$

and

$$\begin{aligned} \Im \Delta^+(R, \tau) &= -\frac{1}{8\pi^2 R} P \left(\frac{1}{\frac{R}{c_0} - \tau} + \frac{1}{\frac{R}{c_0} + \tau} \right) \\ &= -\frac{c_0}{4\pi^2} P \frac{1}{R^2 - (c_0\tau)^2}. \end{aligned} \quad (24.9)$$

Essentially, the quantity

$$\Delta_{\text{JP}}(R, \tau) = \frac{1}{4\pi R} \left[\delta\left(\frac{R}{c_0} + \tau\right) - \delta\left(\frac{R}{c_0} - \tau\right) \right] \quad (24.10)$$

is the original Jordan–Pauli function [358]. As such, it is just the difference between the Huygens scalar propagators $g(R, -\tau)$ and $g(R, \tau)$; see (2.18).

24.2 Free-Field Commutators for Fields Taken at Different Space–Time Points

If two observables $\hat{O}_1$ and $\hat{O}_2$ do not commute it is not possible to find a common basis (complete set of eigenvectors) for $\hat{O}_1$ and $\hat{O}_2$. The physical properties (variables) associated with the two observables therefore cannot be measured independently of one another. Because of this, it is of importance to know the various commutators between the transverse field operators $\hat{\mathbf{E}}_{\text{T}}$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{A}}_{\text{T}}$. In the present section we shall study the commutators for free fields taken at different space–time points. Since the commutator of $\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t)$ and $\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}', t')$ is of particular importance in near-field electrodynamics, we shall examine this commutator first.

For free fields the destruction and creation operators involve time in the Heisenberg picture as indicated in (23.43) and (23.44), and the expressions for the associated field operators $\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t)$, $\hat{\mathbf{B}}(\mathbf{r}, t)$ and $\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)$, follow by insertion in (23.47)–(23.49). With the help of the commutator relations in (23.41) and (23.42) one easily gets

$$\left[\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}', t') \right] = \frac{\hbar}{2i\epsilon_0 L^3} \sum_{q,s} \epsilon_{qs} \epsilon_{qs} \left[e^{i(q \cdot \mathbf{R} - c_0 q \tau)} + c.c. \right], \quad (24.11)$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and $\tau = t - t'$. As expected, the result in (24.11) shows that the free field commutator is translational invariant in space and time. All other free-field commutators exhibit the same invariance, of course. The relation in (15.52) reduces (24.11) to

$$\begin{aligned} [\hat{A}_T(\mathbf{r}, t), \hat{E}_T(\mathbf{r}', t')] &= \frac{\hbar}{2i\epsilon_0 L^3} \sum_q (U - \kappa\kappa) \left[e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} + c.c. \right] \\ &\rightarrow \frac{\hbar}{2i\epsilon_0} \int_{-\infty}^{\infty} (U - \kappa\kappa) \left[e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} + c.c. \right] \frac{d^3 q}{(2\pi)^3}, \end{aligned} \quad (24.12)$$

where the last expression holds in the limit $L \rightarrow \infty$. The result in (24.12) is conveniently expressed in terms of the massless Jordan–Pauli scalar propagator. Thus, from (24.1)–(24.3) and (24.5) the reader may verify that

$$\frac{\partial}{\partial \tau} \Delta_{JP}(R, \tau) = -\frac{c_0^2}{2} \int_{-\infty}^{\infty} \left[e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} + c.c. \right] \frac{d^3 q}{(2\pi)^3 q^2}. \quad (24.13)$$

Furthermore, one has

$$\int_{-\infty}^{\tau} \Delta^+(R, \tau') d\tau' = \frac{1}{2} \int_{-\infty}^{\infty} e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} \frac{d^3 q}{(2\pi)^3 q^2}, \quad (24.14)$$

provided the integral is regularized by a convergence factor $\exp(-q\eta)$, $\eta \rightarrow 0^+$, so that the contribution from the lower limit gives zero. From (24.14) and its complex conjugate a simple calculation gives

$$\nabla \nabla \int_{-\infty}^{\tau} \Delta_{JP}(R, \tau') d\tau' = -\frac{1}{2} \int_{-\infty}^{\infty} \kappa\kappa \left[e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} + c.c. \right] \frac{d^3 q}{(2\pi)^3}, \quad (24.15)$$

since $\nabla \nabla = \nabla_R \nabla_R$. Use of (24.13) and (24.15) immediately shows that

$$[\hat{A}_T(\mathbf{r}, t), \hat{E}_T(\mathbf{r}', t')] = \frac{i\hbar}{\epsilon_0} \left[c_0^{-2} U \frac{\partial}{\partial \tau} \Delta_{JP}(R, \tau) - \nabla \nabla \int_{-\infty}^{\tau} \Delta_{JP}(R, \tau') d\tau' \right]. \quad (24.16)$$

An explicit expression for the commutator in (24.16) now can be obtained using (24.10). Although the calculation is straightforward it may be helpful for the reader to give a few of the intermediate results. Letting δ' and δ'' stand for the first and second derivatives of the delta function with respect to its argument one has

$$\frac{\partial}{\partial \tau} \Delta_{JP}(R, \tau) = \frac{c_0^2}{4\pi R} [\delta'(R + c_0 \tau) + \delta'(R - c_0 \tau)]. \quad (24.17)$$

The time-integral of Δ_{JP} gives

$$\int_{-\infty}^{\tau} \Delta_{\text{JP}}(R, \tau') d\tau' = \frac{1}{4\pi R} [\theta(c_0\tau + R) - \theta(c_0\tau - R)], \quad (24.18)$$

where θ again is the Heaviside step function. Since the result in (24.18) only depends on the numerical magnitude of R , one may use the easily derived formula

$$\nabla \nabla f(R) = \left(U - \hat{R} \hat{R} \right) \frac{1}{R} \frac{df(R)}{dR} + \hat{R} \hat{R} \frac{df(R)}{dR} \quad (24.19)$$

to calculate the last term in (24.16). On basis of the result

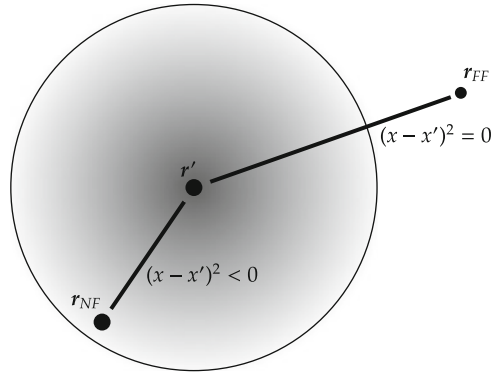
$$\begin{aligned} \nabla \nabla (R^{-1} \theta(c_0\tau \pm R)) &= \pm \hat{R} \hat{R} \frac{1}{R} \delta'(R \pm c_0\tau) \\ &+ \left(U - 3\hat{R} \hat{R} \right) \left[\pm \frac{1}{R^2} \delta(R \pm c_0\tau) - \frac{1}{R^3} \theta(c_0\tau \pm R) \right], \end{aligned} \quad (24.20)$$

one finally is led to the following explicit expression for the commutator between $\hat{A}_{\text{T}}$ and $\hat{E}_{\text{T}}$ taken at different space–time points:

$$\begin{aligned} [\hat{A}_{\text{T}}(\mathbf{r}, t), \hat{E}_{\text{T}}(\mathbf{r}', t')] &= \frac{i\hbar}{4\pi\epsilon_0} \left\{ \left(U - \hat{R} \hat{R} \right) \frac{1}{R} (\delta'(R + c_0\tau) + \delta'(R - c_0\tau)) \right. \\ &- \left(U - 3\hat{R} \hat{R} \right) \left[\frac{1}{R^2} (\delta(R + c_0\tau) + \delta(R - c_0\tau)) \right. \\ &\left. \left. + \frac{1}{R^3} (\theta(c_0\tau - R) - \theta(c_0\tau + R)) \right] \right\}. \end{aligned} \quad (24.21)$$

For a given $\tau = t - t' (\neq 0)$ the commutator contains terms which decay as R^{-1} , R^{-2} and R^{-3} as a function of the distance between the space points $\mathbf{r}$ and $\mathbf{r}'$. The mid- and far-field terms are functions of $\delta(R \pm c_0\tau)$ and their first derivatives, respectively. Outside the forward and backward light cones defined by $R = c_0\tau$ and $R = -c_0\tau$ the physical variables $\hat{A}_{\text{T}}$ and $\hat{E}_{\text{T}}$ thus can be measured independently of each other for mid- and far-field separations. The presence of the step functions $\theta(c_0\tau \mp R)$ shows that commutator between $\hat{A}_{\text{T}}$ and $\hat{E}_{\text{T}}$ is different from zero outside the light cones, but only for near-field separations of the space points $\mathbf{r}$ and $\mathbf{r}'$. The factor $\theta(c_0\tau - R) - \theta(c_0\tau + R)$ is zero for time-like separations ($c_0|t - t'| > R$) and equal to -1 for space-like separations ($c_0|t - t'| < R$), and this indicates a correlation between space-like events in the near-field domain; see Fig. 24.1. This does not imply that information can be transferred with superluminal speed between points separated at near-field distances. At this stage it is interesting to recall the fact that also the transverse propagator for the electric field ($\mathbf{G}_{\text{T}}(\mathbf{R}, \tau)$) has a space-like near-field part; (14.34).

Fig. 24.1 For far-field (FF) separations, $r_{\text{FF}} = r'$, the free-field commutator $[\hat{A}_{\text{T}}(r_{\text{FF}}, t), \hat{E}_{\text{T}}(r', t')]$ is nonvanishing only on the light cone, i.e., for $(x - x')^2 = 0$. For space points with near-field (NF) separation, $r_{\text{NF}} = r'$, $[\hat{A}_{\text{T}}(r_{\text{NF}}, t), \hat{E}_{\text{T}}(r', t')]$ is different from zero only in front of the light cone, i.e., for $(x - x')^2 < 0$



Let us turn the attention now towards the free-field commutators

$$[\hat{E}_{\text{T}}(r, t), \hat{E}_{\text{T}}(r', t')] = c_0^2 [\hat{B}(r, t), \hat{B}(r', t')]. \quad (24.22)$$

Starting from the expansion for $\hat{E}_{\text{T}}$ given in (23.49) plus the commutator relations in (23.41) and (23.42), one obtains in the continuum limit

$$[\hat{E}_{\text{T}}(r, t), \hat{E}_{\text{T}}(r', t')] = \frac{\hbar c_0}{2\epsilon_0} \int_{-\infty}^{\infty} (U - \kappa \kappa) q \left[e^{i(q \cdot R - c_0 q \tau)} - c.c. \right] \frac{d^3 q}{(2\pi)^3}. \quad (24.23)$$

The result in (24.23) may be expressed in terms of the function Δ^+ (24.1) as follows:

$$[\hat{E}_{\text{T}}(r, t), \hat{E}_{\text{T}}(r', t')] = -\frac{\hbar}{\epsilon_0} \left[i \left(U \frac{1}{c_0^2} \frac{\partial^2}{\partial \tau^2} - \nabla \nabla \right) \Delta^+(R, \tau) - c.c. \right], \quad (24.24)$$

or equivalently in the form

$$[\hat{E}_{\text{T}}(r, t), \hat{E}_{\text{T}}(r', t')] = \frac{2i\hbar}{\epsilon_0} \left(\nabla \nabla - U c_0^{-2} \frac{\partial^2}{\partial \tau^2} \right) \Re \Delta^+(R, \tau). \quad (24.25)$$

An explicit expression for the commutator now can be obtained inserting the formula for $\Re \Delta^+(R, \tau)$ given in (24.8) into (24.25). The details of the subsequent calculation is left as an exercise for the reader, and here I just quote the final result, namely

$$\begin{aligned} [\hat{E}_{\text{T}}(r, t), \hat{E}_{\text{T}}(r', t')] = & \frac{\hbar c_0}{4\pi i \epsilon_0} \left\{ \left(U - \hat{R} \hat{R} \right) \frac{1}{R} (\delta''(R + c_0 \tau) - \delta''(R - c_0 \tau)) \right. \\ & - \left(U - 3 \hat{R} \hat{R} \right) \left[\frac{1}{R^2} (\delta'(R + c_0 \tau) - \delta'(R - c_0 \tau)) \right. \\ & \left. \left. - \frac{1}{R^3} (\delta(R + c_0 \tau) - \delta(R - c_0 \tau)) \right) \right] \right\}. \end{aligned} \quad (24.26)$$

The commutators in (24.22) hence are zero outside the forward and backward light cones, and the far-, mid- and near-field parts contains δ'' , δ' and δ , respectively. Since $\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) = -\partial \hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t)/\partial t$, and $\tau = t - t'$,

$$-\frac{\partial}{\partial \tau} [\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}', t')] = [\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{E}}_{\text{T}}(\mathbf{r}', t')]. \quad (24.27)$$

By acting in the right-hand-side of (24.21) with the differential operator $-\partial/\partial \tau$ one immediately obtains the expression in (24.26).

To determine the explicit expression for the free-field commutator

$$\begin{aligned} & [\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t')] \\ &= \frac{\hbar}{2\epsilon_0 c_0 L^3} \sum_{q,s} \omega_q [\boldsymbol{\epsilon}_{qs} \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} - \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} e^{-i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)}], \end{aligned} \quad (24.28)$$

we make use of the following result for the summation over the polarization states:

$$\sum_s \boldsymbol{\epsilon}_{qs} \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} = - \sum_s \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} = -\boldsymbol{\kappa} \times (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}) = -\boldsymbol{\kappa} \times \mathbf{U} = -\mathbf{U} \times \boldsymbol{\kappa}. \quad (24.29)$$

In the continuum limit one therefore obtains

$$[\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t')] = -\mathbf{U} \times \left\{ \frac{\hbar}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{q} [e^{i(\mathbf{q} \cdot \mathbf{R} - c_0 q \tau)} - c.c.] \frac{d^3 q}{(2\pi)^3} \right\}. \quad (24.30)$$

In terms of the real part of $\Delta^+(R, \tau)$, the commutator can be expressed in the compact form

$$[\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t')] = \frac{2\hbar}{i\epsilon_0 c_0^2} \mathbf{U} \times \left[\frac{\partial}{\partial \tau} \nabla \Re \Delta^+(R, \tau) \right], \quad (24.31)$$

and by inserting here the relation in (24.8), one is led to the final expression

$$\begin{aligned} [\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t')] &= \frac{\hbar}{4\pi i \epsilon_0} \mathbf{U} \times \hat{\mathbf{R}} \left[\frac{1}{R} (\delta''(R + c_0 \tau) + \delta''(R - c_0 \tau)) \right. \\ &\quad \left. - \frac{1}{R^2} (\delta'(R + c_0 \tau) + \delta'(R - c_0 \tau)) \right]. \end{aligned} \quad (24.32)$$

The commutator between the transverse electric and magnetic fields is zero outside the light cones, and it has no near-field (R^{-3}) part.

24.3 Field Commutators in the Presence of Field–Matter Interaction

24.3.1 Equal-Time Commutators

In the Schrödinger picture, the field operators $\hat{A}_T(\mathbf{r})$, $\hat{B}(\mathbf{r})$ and $\hat{E}_T(\mathbf{r})$ are given by (23.47)–(23.49). The corresponding operators in the Heisenberg picture, viz., $\hat{A}_T(\mathbf{r}, t)$, $\hat{B}(\mathbf{r}, t)$ and $\hat{E}_T(\mathbf{r}, t)$ are obtained from (23.47)–(23.49) by the replacements $\hat{a}_{qs}(0) \Rightarrow \hat{a}_{qs}(t)$, $\hat{a}_{qs}^\dagger(0) \Rightarrow \hat{a}_{qs}^\dagger(t)$, and in the presence of field–matter interactions the time dependent annihilation and creation operators satisfy the dynamical equations in (23.137) and (23.138). With the help of the equal-time commutator relations in (23.45) and (23.46) the reader may convince herself that the equal-time commutator between $\hat{A}_T(\mathbf{r}, t)$ and $\hat{E}_T(\mathbf{r}', t)$ at two different space points is given by

$$\begin{aligned} \left[\hat{A}_T(\mathbf{r}, t), \hat{E}_T(\mathbf{r}', t) \right] &= \frac{\hbar}{2i\epsilon_0} \int_{-\infty}^{\infty} (U - \kappa\kappa) (e^{i\mathbf{q}\cdot\mathbf{R}} + c.c.) \frac{d^3q}{(2\pi)^3} \\ &= \frac{\hbar}{2i\epsilon_0} (\delta_T(\mathbf{R}) + \delta_T(-\mathbf{R})). \end{aligned} \quad (24.33)$$

Since the transverse delta function is an even function of $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ one has

$$\left[\hat{A}_T(\mathbf{r}, t), \hat{E}_T(\mathbf{r}', t) \right] = \frac{\hbar}{i\epsilon_0} \delta_T(\mathbf{R}). \quad (24.34)$$

With or without field–matter interaction the fields $A_T(\mathbf{r}, t)$ and $E_T(\mathbf{r}', t)$ thus are correlated at near-field distances, and the equal-time correlation is time independent, as one perhaps might have expected.

The connection in (24.27) of course holds in the presence of field–matter interactions, and since the right-hand-side of (24.34) does not depend on time one obtains

$$\left[\hat{E}_T(\mathbf{r}, t), \hat{E}_T(\mathbf{r}', t) \right] = \left[\hat{B}(\mathbf{r}, t), \hat{B}(\mathbf{r}', t) \right] = \mathbf{0}. \quad (24.35)$$

It is obvious that the equal-time commutator between the transverse electric and magnetic fields must be given by (24.30) setting $\tau = 0$ even in the presence of field–matter interactions. Thus,

$$\left[\hat{E}_T(\mathbf{r}, t), \hat{B}(\mathbf{r}', t) \right] = -U \times \left[\frac{\hbar}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{q} (e^{i\mathbf{q}\cdot\mathbf{R}} - e^{-i\mathbf{q}\cdot\mathbf{R}}) \frac{d^3q}{(2\pi)^3} \right]. \quad (24.36)$$

A substitution $\mathbf{q} \Rightarrow -\mathbf{q}$ in the integral containing the $\exp(-i\mathbf{q} \cdot \mathbf{R})$ -factor leads to

$$\left[\hat{E}_T(\mathbf{r}, t), \hat{B}(\mathbf{r}', t) \right] = -U \times \left[\frac{\hbar}{\epsilon_0} \int_{-\infty}^{\infty} \mathbf{q} e^{i\mathbf{q}\cdot\mathbf{R}} \frac{d^3q}{(2\pi)^3} \right] \quad (24.37)$$

or equivalently

$$\left[\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t), \hat{\mathbf{B}}(\mathbf{r}', t) \right] = \frac{i\hbar}{\epsilon_0} \mathbf{U} \times \nabla \delta(\mathbf{R}), \quad (24.38)$$

where $\delta(\mathbf{R})$ is the Dirac delta function, which plane-wave expansion is given by (4.23). The result in (24.38) shows that $\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)$ and $\hat{\mathbf{B}}(\mathbf{r}', t)$ are correlated only when $\mathbf{r} = \mathbf{r}'$.

24.3.2 Weighted Average Values of Fields and Commutators

The measurement of the transverse field at a space–time point requires placing a test charge at that point [316, 317]. Even if the test charge was a point entity one would never be able to localize it completely in space–time (see Fig. 24.2). Independent of how the field measurement is carried out one only can obtain a (weighted) average of the field over a certain space–time region. The impossibility of measuring local fields in a sense manifests itself through the occurrence of delta functions in the various field commutators we have calculated above. To be a bit more specific let us consider the transverse part $\hat{\mathbf{E}}_{\text{T}}$ of the electric field operator, and then introduce a related mean-field operator

$$\bar{\mathbf{E}}_{\text{T}}(x) = \int_{-\infty}^{\infty} f(x') \hat{\mathbf{E}}_{\text{T}}(x - x') d^4 x', \quad (24.39)$$

where $f(x')$ is a real weighting function, which effectively only differs from zero in a small (finite) space–time volume surrounding the space–time point x , and which

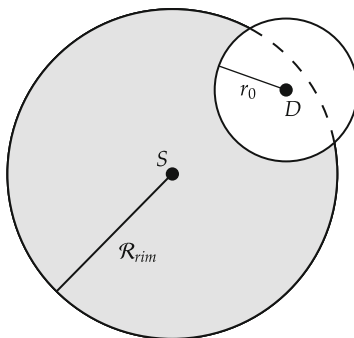


Fig. 24.2 In order to measure the transverse electromagnetic field at a certain point in the rim zone of a source (S) one might imagine to place a point-like test particle (detector (D)) in this point. In all cases only some weighted averaged value of the field, say over a volume of linear extension r_0 , is obtainable. With S and D in near-field contact at best only the weighted average of the self-consistent field (not the source field) is experimentally measurable. The limits put on the accuracy of field measurements have been discussed in detail in two famous papers by Bohr and Rosenfeld [316, 317]

is normalized according to

$$\int_{-\infty}^{\infty} f(x) d^4x = 1. \quad (24.40)$$

In order to avoid overloading the notation no operator symbol $\wedge$ is placed on top of $\bar{E}_T(x)$. Rather than considering the consequences of the complete space–time averaging process, let us neglect the time averaging and just consider the spatial mean field operator

$$\bar{E}_T(\mathbf{r}, t) = \int_{-\infty}^{\infty} f(\boldsymbol{\rho}) \bar{E}_T(\mathbf{r} - \boldsymbol{\rho}, t) d^3\rho. \quad (24.41)$$

For simplicity we assume that the bell-shaped real function $f(\boldsymbol{\rho})$ depends only on $\rho = |\boldsymbol{\rho}|$. Again, the weight function is normalized, i.e.,

$$\int_{-\infty}^{\infty} f(\rho) d^3\rho = 1. \quad (24.42)$$

Using the expansion for $\hat{E}_T$ given in (23.49), the mean field operator becomes in the Heisenberg picture

$$\bar{E}_T(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0} \right)^{1/2} \hat{a}_{qs}(t) f(\mathbf{q}) \epsilon_{qs} e^{i\mathbf{q} \cdot \mathbf{r}} + h.c., \quad (24.43)$$

where

$$f(\mathbf{q}) = \int_{-\infty}^{\infty} f(\boldsymbol{\rho}) e^{-i\mathbf{q} \cdot \boldsymbol{\rho}} d^3\rho \quad (24.44)$$

is the Fourier integral transform of the weight function. For the isotropic $f(\rho)$ one has

$$f(q) = \frac{4\pi}{q} \int_0^{\infty} \rho f(\rho) \sin(q\rho) d\rho. \quad (24.45)$$

If the effective width of $f(\rho)$ is r_0 , $f(q)$ tends to zero when $q \gg r_0^{-1}$. The averaging of the field over a volume of linear extend r_0 about the point $\mathbf{r}$ thus is equivalent to introducing a cutoff function $f(q)$ in the mode expansion of the field given in (24.43).

24.3.3 *Quantum Mechanical Mean Value and Variance of the Mean Field*

It is well known that the quantum theory of radiation predicts that even in vacuum there is at every point in space an electromagnetic field with zero mean value and infinite variance. In a measurement, where the field always is averaged over some (small) region of space, the variance will remain finite, as we shall see now.

Since, for all $(\mathbf{q}, s)$ -modes one has

$$\hat{a}_{qs}|0\rangle = \langle 0|\hat{a}_{qs}^\dagger = 0, \quad (24.46)$$

it is clear that the quantum mechanical mean value of the transverse mean-field operator $\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)$ vanishes identically in the global vacuum state $(|0\rangle)$, i.e.,

$$\langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle = 0. \quad (24.47)$$

To determine the variance of $\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)$, we make use of the result that the mean values in the vacuum of the products $\hat{a}_{\mathbf{q}'s'}(t)\hat{a}_{\mathbf{q}s}(t)$, $\hat{a}_{\mathbf{q}'s'}(t)\hat{a}_{\mathbf{q}s}^\dagger(t)$ and $\hat{a}_{\mathbf{q}'s'}^\dagger(t)\hat{a}_{\mathbf{q}s}(t)$ all give zero, and that

$$\langle 0|\hat{a}_{\mathbf{q}'s'}(t)\hat{a}_{\mathbf{q}s}^\dagger(t)|0\rangle = \delta_{\mathbf{q}'s'}\delta_{\mathbf{q}s} = \delta_{\mathbf{q}\mathbf{q}'}\delta_{ss'}. \quad (24.48)$$

With the help of these facts one obtains the following mean value of the square of the mean-field operator:

$$\langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) \cdot \bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle = 2L^{-3} \sum_{\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{2\epsilon_0} f^2(\mathbf{q}). \quad (24.49)$$

The factor of 2 in front of L^{-3} comes from the summation over the two polarization states. In the continuum limit one thus finds

$$\langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) \cdot \bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle = \frac{\hbar c_0}{2\pi^2\epsilon_0} \int_0^\infty q^3 f^2(q) dq. \quad (24.50)$$

The root-mean-square deviation of the transverse mean field in the vacuum state, viz.,

$$\Delta \bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) \equiv \left[\langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) \cdot \bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle - \langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle \cdot \langle 0|\bar{\mathbf{E}}_{\text{T}}(\mathbf{r}, t)|0\rangle \right]^{1/2}, \quad (24.51)$$

hence is finite if the weight function tends sufficiently rapidly towards zero for $q \rightarrow \infty$. For the local field the quantity

$$\langle 0|\mathbf{E}_{\text{T}}(\mathbf{r}, t) \cdot \mathbf{E}_{\text{T}}(\mathbf{r}, t)|0\rangle = \frac{\hbar c_0}{2\pi^2\epsilon_0} \int_0^\infty q^3 dq \quad (24.52)$$

diverges as already mentioned. The relations in (24.46) implies that also the local field has zero quantum mechanical mean value in the global vacuum state.

24.4 Contour Integral Representations of Covariant Scalar Propagators

24.4.1 The Jordan–Pauli Propagator

It is now postulated that the Jordan–Pauli scalar propagator, given in (24.5) in terms of the $\Delta^+(x)$ -function (24.1) and its complex conjugate $\Delta^-(x)$, can be written in the Lorentz-invariant form

$$\Delta_{JP}(x) = \frac{c_0}{i} \int_{-\infty}^{\infty} \delta(q_\mu q^\mu - Q_C^2) \operatorname{sgn}(q^0) e^{-iq_\mu x^\mu} \frac{dq^0 d^3q}{(2\pi)^3}. \quad (24.53)$$

In Sect. 14.6 it was shown that the Huygens propagator $\delta(R/c_0 - \tau)/(4\pi R)$ is relativistically covariant. The same applies to the propagator $\delta(R/c_0 + \tau)/(4\pi R)$, and since $\Delta_{JP}(x)$ is just the difference between these propagators (see (24.10)), the Jordan–Pauli propagator is Lorentz invariant. Since proper Lorentz transformations do not interchange past and future the signum function $\operatorname{sgn}(q^0)$ [$\operatorname{sgn}(q^0) = +1$ if $q^0 > 0$ and -1 if $q^0 < 0$] is Lorentz invariant, and the expression on the right side of (24.53) hence is manifestly covariant. In order to prove that the expression also equals the Jordan–Pauli propagator, the delta function is transformed as follows:

$$\begin{aligned} \delta(q_\mu q^\mu - Q_C^2) &= \delta[-q^2 + (q^0)^2 - Q_C^2] = \delta\left[-\left(\frac{\omega_q}{c_0}\right) + (q^0)^2\right] \\ &= \frac{c_0}{2\omega_q} \left[\delta\left(q^0 - \frac{\omega_q}{c_0}\right) + \delta\left(q^0 + \frac{\omega_q}{c_0}\right) \right]. \end{aligned} \quad (24.54)$$

The second rewriting in (24.54) is obtained by means of the relativistic dispersion relation in (24.2), remembering that Q_C is the Compton wave number (see (16.63)). The last form in (24.54) allows one to carry out the integration over q^0 in (24.53). Hence, we obtain

$$\Delta_{JP}(x) = \frac{c_0^2}{2i} \left[\int_{-\infty}^{\infty} e^{i(q \cdot R - \omega_q \tau)} \frac{d^3q}{(2\pi)^3 \omega_q} - \int_{-\infty}^{\infty} e^{i(q \cdot R + \omega_q \tau)} \frac{d^3q}{(2\pi)^3 \omega_q} \right]. \quad (24.55)$$

The first term in (24.55) is just $\Delta^+(x)$, see (24.1), and by a variable substitution $q \Rightarrow -q$ in the second integral the reader may convince himself that the second term is precisely $\Delta^-(x) = (\Delta^+(x))^*$. Altogether it has thus been demonstrated that the expression in (24.53) is an integral representation for the Jordan–Pauli propagator.

A particularly useful way of representing the functions $\Delta^+(x)$, $\Delta^-(x)$ and $\Delta_{JP}(x)$ is as contour integrals in a complex q^0 -plane. All three functions thus may be obtained from the common form

$$\Delta(x) = -c_0 \int_C \frac{e^{-iq_\mu x^\mu}}{q_\mu q^\mu - Q_C^2} \frac{dq^0 d^3q}{(2\pi)^4}, \quad (24.56)$$

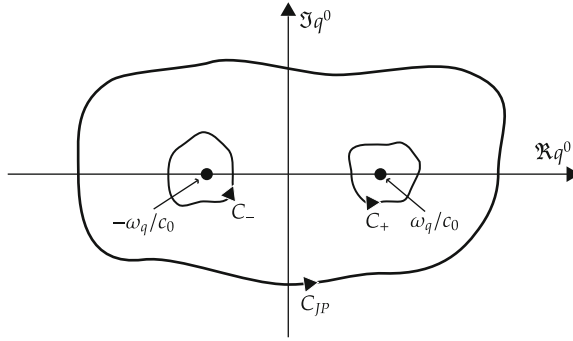


Fig. 24.3 Schematic illustration showing the contours in the complex q^0 -plane used to determine the functions $\Delta^+(x)$, $\Delta^-(x)$, and $\Delta_{JP}(x)$ from the integral representation given in (24.56). First-order poles are located on the real axis at $q^0 = \pm\omega_q/c_0$. Integration along the contour C_{JP} gives one the Jordan–Pauli propagator, and the integrations along C_+ and C_- lead to $\Delta^+(x)$ and $\Delta^-(x)$, respectively

as we now shall see. The contour in the complex q^0 -plane is indicated by the C at the foot of the integral sign. By rewriting (24.56) as follows

$$\Delta(x) = c_0 \int_{-\infty}^{\infty} \left[\int_C \frac{e^{-iq_\mu x^\mu}}{\left(\frac{\omega_q}{c_0} - q^0\right)\left(\frac{\omega_q}{c_0} + q^0\right)} \frac{dq^0}{2\pi} \right] \frac{d^3q}{(2\pi)^3}, \quad (24.57)$$

it appears that the integrand has first-order poles on the real q^0 -axis at $q^0 = \pm\omega_q/c_0$. By performing integrations along the contours C^+ and C^- shown in Fig. 24.3, one picks up the residues from the poles located at $+\omega_q/c_0$ and $-\omega_q/c_0$, respectively. Residue calculations in turn show that $\Delta(x) = \Delta^+(x)$ for the C^+ -contour, and $\Delta(x) = \Delta^-(x) = (\Delta^+(x))^*$ for the C^- -contour, remembering the definition of $\Delta^+(x)$ (24.1). With a contour C_{JP} enclosing both poles (see Fig. 24.3), the integral in (24.56) equals the Jordan–Pauli propagator, i.e., $\Delta(x) = \Delta_{JP}(x)$.

24.4.2 The Feynman Propagator

We shall now realize that the Feynman scalar propagator, also called the meson propagator, can be represented by a contour integral similar to the one for the Δ^+ , Δ^- and Δ_{JP} functions, namely

$$\Delta_F(x) = c_0 \int_{C_F} \frac{e^{-iq_\mu x^\mu}}{q_\mu q^\mu - Q_C^2} \frac{dq^0 d^3q}{(2\pi)^4}. \quad (24.58)$$

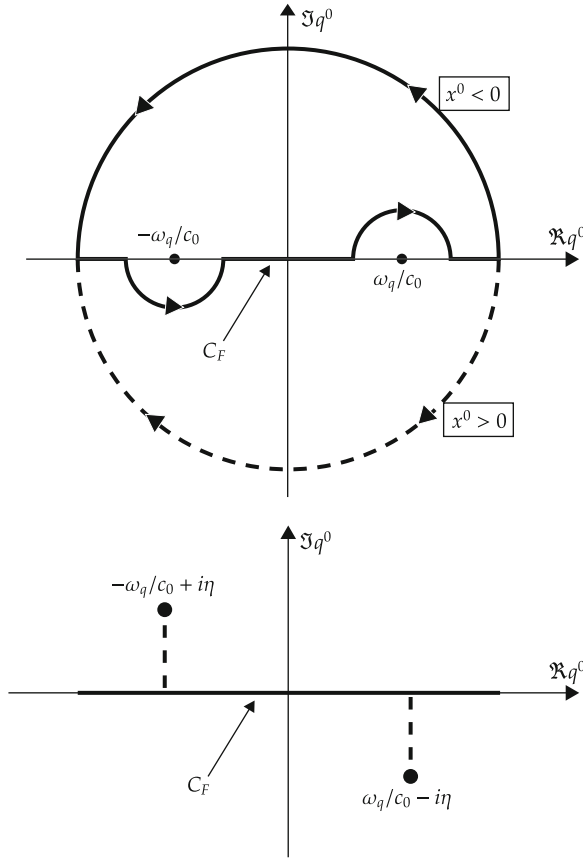


Fig. 24.4 The Feynman scalar propagator, $\Delta_F(x)$, can be represented by the contour (C_F) integral given in (24.58), and a graphical illustration of the relevant contours in the complex q^0 -plane is shown here. *Top figure:* The contour runs along the real axis circulating the first-order poles located on the real axis at $q^0 = \pm\omega_q/c_0$ as shown. For $x^0 < 0$ the contour is closed by a semicircle in the upper halfplane. For $x^0 > 0$, the semicircle lies in the lower halfplane. *Bottom figure:* Alternative determination of $\Delta_F(x)$ with the poles slightly displaced from the real axis, as shown

Note that the integral forms for $\Delta(x)$ (24.56) and $\Delta_F(x)$ (24.58) differ from each other by a minus sign only. The meson propagator in (24.4) is manifestly covariant, and so is the integral in (24.58). The contour C_F for the meson propagator runs for both $x^0 = c_0\tau > 0$ and $x^0 < 0$ along the real q^0 -axis circulating the poles located at $q^0 = \pm\omega_q/c_0$ in infinitely small semicircles, as shown in Fig. 24.4. For $x^0 > 0$ the contour is closed by means of a semicircle of infinitely large radius located in the lower half of the complex q^0 -plane. The reason that the contour must be closed in the lower halfplane stems from the fact that the factor

$$= \exp(-iq_0x^0) = \exp(-ix^0\Re q^0) \exp(x^0\Im q^0) \quad (24.59)$$

in the integrand of (24.58) for $x^0 > 0$ vanishes exponentially for $\Im q^0 \rightarrow -\infty$. The contribution from the large semicircle, therefore, gives zero in the limit where its radius becomes infinitely large. Thanks to the minus sign in front of the integral in (24.56), and the fact that the contours C_+ and C_F are circulated in opposite directions (C_F clockwise), it follows that $\Delta_F(x) = \Delta^+(x)$ for $\tau > 0$, in agreement with (24.4). For $x^0 < 0$, the contour is closed in the upper half of the complex q^0 -plane by a semicircle of infinite radius. Since the integration now runs counter-clockwise along the contour the reader may convince himself that $\Delta_F(x) = -\Delta^-(x)$ for $\tau < 0$, again in agreement with the definition in (24.4). This concludes our connection of the contour integral(s) in (24.58) to (24.4).

It is well known that instead of deforming the contour along the real q^0 -axis, as shown in Fig. 24.4, the poles can be moved an infinitesimal distance η up and down from the real axis (Fig. 24.4). The meson propagator then is obtained from the integral representation

$$\Delta_F(x) = c_0 \int_{C_F} \frac{e^{-iq_\mu x^\mu}}{q_\mu q^\mu - Q_C^2 + i\epsilon} \frac{dq^0 d^3q}{(2\pi)^4}, \quad (24.60)$$

where $\epsilon = 2\eta\omega_q/c_0 \rightarrow 0^+$. The q^0 -integration now is carried out along the whole real axis.

The Feynman photon propagator, which is introduced and discussed in Chap. 30, has an integral representation closely related to the one in (24.60). The Feynman photon propagator contains contributions not only from the transverse photons, but also from the longitudinal and scalar photons which are so important in near-field quantum electrodynamics.

Chapter 25

Electrodynamics in the Poincaré Gauge

In the near-field zone of matter, the dynamics of particles and field are coupled. As we have seen in previous chapters, this coupling can be described in various manners. In the covariant approach the near-field electrodynamics is considered as a coupling of transverse photons to longitudinal and scalar photons. The L- and S-photons are mutually coupled through the Lorenz gauge condition. A unitary transformation allows one to replace these last two photon types by gauge and near-field photons. From a physical point of view the presence of the L- and S-photons (or equivalently the NF- and G-photons) is not needed since all observable effects of the photons relate to the longitudinal part of the electric field. As we know, the longitudinal field is completely described in every space-time point in terms of the dynamics of the particle position variables. Up to this point we have identified the embryo state of the transverse photons with the state of the transverse part of the electromagnetic field. Although this identification may appear natural, physically it is just one choice among infinitely many other choices, which in the final analysis all lead to the same conclusion in regard to observational predictions. From a field-quantized perspective it is useful, but not necessary, to link the photon embryo to the chosen set of conjugate “position” and “momentum” variables for the electromagnetic field. In the Coulomb gauge, the conjugate field variables are the vector potential, $\mathbf{A}_T(\mathbf{r})$, and its time derivative multiplied by the vacuum permittivity, $\epsilon_0 \dot{\mathbf{A}}_T(\mathbf{r})$. A change of gauge in general results in new conjugate field variables, and thus in a new choice for what is called the photon embryo. In the present chapter we shall consider one particular gauge, namely the so-called Poincaré gauge. The gauge function which brings one from the initial (Coulomb) gauge to the Poincaré gauge relates closely to a specific choice for the generalized polarization. In the Poincaré gauge the conjugate field variables are the transverse part of the vector potential, $\mathbf{A}_T(\mathbf{r})$, and the negative of the transverse part of the electric displacement field, $-\mathbf{D}_T(\mathbf{r})$. The Poincaré gauge is of particular interest for the description of the near-field electrodynamics attached to atomic and mesoscopic sources, as the reader will learn later on.

25.1 The Poincaré Gauge

Let us assume that we start from the Coulomb gauge, and let us denote the potentials in this gauge by $\mathbf{A}(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$. In the Coulomb gauge, the vector potential is purely transverse, i.e., $\mathbf{A}(\mathbf{r}, t) = \mathbf{A}_T(\mathbf{r}, t)$. Transformations to other gauges ($\mathbf{A}'(\mathbf{r}, t), \phi'(\mathbf{r}, t)$) are effectuated by the arbitrary gauge function $\chi(\mathbf{r}, t)$ in the manner described in (2.11) and (2.12). The transformation to the Poincaré gauge is obtained by the specific choice (superscript P for Poincaré)

$$\chi^P(\mathbf{r}, t) = - \int_0^1 \mathbf{r} \cdot \mathbf{A}_T(u\mathbf{r}, t) du, \quad (25.1)$$

where u is a real variable. Although it is useful here to assume that the initial gauge is the Coulomb gauge, the gauge function in (25.1) is independent of the initial gauge choice because the transverse part of the vector potential, $\mathbf{A}_T(\mathbf{r}, t)$, is gauge invariant. The reason for making the choice in (25.1) will soon become clear to the reader. In the new gauge, the vector potential is no longer transverse. One finds the longitudinal part of the vector potential in the Poincaré gauge, $\mathbf{A}_L^P(\mathbf{r}, t)$, from the formula

$$\mathbf{A}_L^P(\mathbf{r}, t) = -\nabla \int_0^1 \mathbf{r} \cdot \mathbf{A}_T(u\mathbf{r}, t) du. \quad (25.2)$$

We now take the scalar product of $\mathbf{r}$ and the vector potential in the Poincaré gauge, viz.,

$$\mathbf{A}^P(\mathbf{r}, t) = \mathbf{A}_T(\mathbf{r}, t) + \mathbf{A}_L^P(\mathbf{r}, t). \quad (25.3)$$

By means of the identity

$$u \frac{\partial}{\partial u} f(u\mathbf{r}) = (\mathbf{r} \cdot \nabla) f(u\mathbf{r}) \quad (25.4)$$

the scalar product can be rewritten as follows:

$$\begin{aligned} \mathbf{r} \cdot \mathbf{A}^P(\mathbf{r}, t) &= \mathbf{r} \cdot \mathbf{A}_T(\mathbf{r}, t) - \int_0^1 (\mathbf{r} \cdot \nabla) (\mathbf{r} \cdot \mathbf{A}_T(u\mathbf{r}, t)) du \\ &= \mathbf{r} \cdot \mathbf{A}_T(\mathbf{r}, t) - \int_0^1 u^{-1} (\mathbf{r} \cdot \nabla) (u\mathbf{r} \cdot \mathbf{A}_T(u\mathbf{r}, t)) du \\ &= \mathbf{r} \cdot \mathbf{A}_T(\mathbf{r}, t) - \int_0^1 \frac{\partial}{\partial u} (u\mathbf{r} \cdot \mathbf{A}_T(u\mathbf{r}, t)) du. \end{aligned} \quad (25.5)$$

Since the last integral is just $\mathbf{r} \cdot \mathbf{A}_T(\mathbf{r}, t)$, one has

$$\mathbf{r} \cdot \mathbf{A}^P(\mathbf{r}, t) = 0. \quad (25.6)$$

In the Poincaré gauge, the vector potential thus is perpendicular to the vector $\mathbf{r}$ everywhere in direct space at all times. For comparison, the vector potential in the Coulomb gauge, $\mathbf{A}^C(\mathbf{r}, t)$ (with superscript C for Coulomb), is normal to the wave vector $\mathbf{q}$ everywhere in reciprocal space, i.e.,

$$\mathbf{q} \cdot \mathbf{A}^C(\mathbf{q}; t) = 0. \quad (25.7)$$

The nice property in (25.6) is not the only interesting thing about the Poincaré gauge. Thus, we shall show now that the scalar and vector potentials are related respectively (and solely) to the electric and magnetic field. Let us first consider the scalar potential. In the Coulomb gauge, the scalar potential $\phi^C(\mathbf{r}, t)$ and the longitudinal electric field $\mathbf{E}_L(\mathbf{r}, t)$ are connected via $\mathbf{E}_L = -\nabla\phi^C$, see (9.88). To within a global constant, ϕ^C thus can be obtained for instance as a line integral

$$\phi^C(\mathbf{r}, t) = - \int_0^1 \mathbf{E}_L(u\mathbf{r}, t) \cdot d(u\mathbf{r}) \quad (25.8)$$

along the straight line joining the origin of the coordinate system to the point $\mathbf{r}$. Since, from (25.1)

$$\frac{\partial}{\partial t} \chi^P(\mathbf{r}, t) = \int_0^1 \mathbf{r} \cdot \mathbf{E}_T(u\mathbf{r}, t) du, \quad (25.9)$$

because $\mathbf{E}_T = -\partial\mathbf{A}_T/\partial t$, one obtains from (2.12), (25.8) and (25.9)

$$\phi^P(\mathbf{r}, t) = - \int_0^1 \mathbf{r} \cdot \mathbf{E}_L(u\mathbf{r}, t) du - \int_0^1 \mathbf{r} \cdot \mathbf{E}_T(u\mathbf{r}, t) du, \quad (25.10)$$

and thus

$$\phi^P(\mathbf{r}, t) = - \int_0^1 \mathbf{r} \cdot \mathbf{E}(u\mathbf{r}, t) du. \quad (25.11)$$

In order to obtain the soughtfor relation between the vector potential in the Poincaré gauge and the magnetic field, we first calculate the gradient of the gauge function in (25.1). In the first step we obtain, leaving out the reference to time from the notation,

$$\nabla\chi^P(\mathbf{r}) = - \int_0^1 \mathbf{A}_T(u\mathbf{r}) du - \sum_i \int_0^1 r_i \nabla A_{T,i}(u\mathbf{r}) du. \quad (25.12)$$

In the second step, the first term of (25.12) is integrated by parts:

$$\begin{aligned} - \int_0^1 \mathbf{A}_T(u\mathbf{r}) du &= -u\mathbf{A}_T(u\mathbf{r}) \Big|_0^1 + \int_0^1 u \frac{\partial}{\partial u} \mathbf{A}_T(u\mathbf{r}) du \\ &= -\mathbf{A}_T(\mathbf{r}) + \int_0^1 (\mathbf{r} \cdot \nabla) \mathbf{A}_T(u\mathbf{r}) du, \end{aligned} \quad (25.13)$$

upon use of (25.4). The vector potential in the Poincaré gauge then is obtained from (2.11), which reads

$$\mathbf{A}^P(\mathbf{r}) = \mathbf{A}_T(\mathbf{r}) + \nabla\chi^P(\mathbf{r}, t), \quad (25.14)$$

since the vector potential is transverse in the Coulomb gauge. By combining (25.12)–(25.14), the reader may convince herself that

$$\mathbf{A}^P(\mathbf{r}) = - \int_0^1 \mathbf{r} \times (\nabla \times \mathbf{A}_T(u\mathbf{r})) du. \quad (25.15)$$

Since

$$\nabla \times \mathbf{A}_T(u\mathbf{r}) = u \nabla_{u\mathbf{r}} \times \mathbf{A}_T(u\mathbf{r}) = u \mathbf{B}(u\mathbf{r}), \quad (25.16)$$

one finally obtains the integral expression

$$\mathbf{A}^P(\mathbf{r}, t) = - \int_0^1 u\mathbf{r} \times \mathbf{B}(u\mathbf{r}, t) du. \quad (25.17)$$

To within a constant the condition in (25.6) defines the Poincaré gauge uniquely. This follows from the fact that in the relation $\mathbf{A}'' = \mathbf{A}' + \nabla\chi$ between two potentials both satisfying (25.6) one must have $\mathbf{r} \cdot \nabla\chi = 0$, and therefore in spherical coordinates $\partial\chi/\partial r = 0$. The function χ is, therefore, equal to its value at the origin everywhere in space, and hence a space-independent constant.

25.2 A Specific Choice for the Generalized Polarization and Magnetization

25.2.1 Polarization Field

We learned from the analysis in Sect. 10.4.1 that one has a certain freedom in the definitions of the transverse parts of the microscopic polarization ($\mathbf{P}_T(\mathbf{r}, t)$) and magnetization ($\mathbf{M}(\mathbf{r}, t)$) fields, cf. (10.45) and (10.46). We shall in the following introduce and study a specific choice for $\mathbf{P}_T(\mathbf{r}, t)$. The choice has a close connection to the gauge function $\chi^P(\mathbf{r}, t)$ (25.1) which, as we shall see in the next section, appears in the transformation from the Coulomb Lagrangian to the Poincaré Lagrangian.

Let us consider an (almost) infinite number of (almost) infinitesimally small electric dipoles aligned along a curve in such a manner that the charge $-q_\alpha$ of one dipole is superimposed on the charge $+q_\alpha$ of the preceding dipole. The tail of the first dipole is assumed to coincide with the origo (O) of our coordinate system, and the

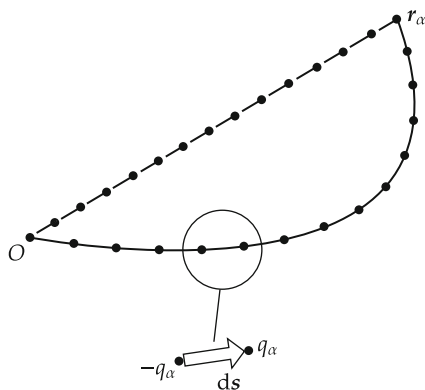


Fig. 25.1 Graphic representation showing that the charge density of a point-particle of charge $+q_\alpha$ located at the position $\mathbf{r}_\alpha$ is equivalent to that of a charge $+q_\alpha$ located at the origo ($\mathcal{O}$) plus a polarization field $\mathbf{P}_\alpha(\mathbf{r})$ (25.18). The generalized polarization field consists of an infinite number of infinitesimally small electric dipoles (dipole moment: $q_\alpha ds$) aligned tangentially along an arbitrary curve with endpoints at $\mathcal{O}$ and $\mathbf{r}_\alpha$. The specific choice corresponding to an alignment along a straight line gives the minimum polarization field

tip of the last dipole has the position vector $\mathbf{r}_\alpha$; see Fig. 25.1. In the limit where one obtains a continuous distribution of point-dipoles, the polarization is given by

$$\mathbf{P}_\alpha(\mathbf{r}) = q_\alpha \int_0^{\mathbf{r}_\alpha} \delta(\mathbf{r} - \mathbf{s}(u_\alpha)) d\mathbf{s}(u_\alpha), \quad (25.18)$$

where $\mathbf{s}(u_\alpha)$ denotes the position vector of a point on the curve considered as a function of say the length u_α of the arc of the curve. The arc length may be normalized so that $0 \leq u_\alpha \leq 1$. The charge density corresponding to a charge $+q_\alpha$ at $\mathcal{O}$ plus the polarization field $\mathbf{P}_\alpha$ is strictly identical to that which corresponds to single charge $+q_\alpha$ at $\mathbf{r}_\alpha$. To describe by the same procedure the charge density of a system of point charges (labeled by α) located at various $\mathbf{r}_\alpha$ -positions one extends the polarization field in (25.18) to the form

$$\mathbf{P}(\mathbf{r}) = \sum_\alpha q_\alpha \int_0^{\mathbf{r}_\alpha} \delta(\mathbf{r} - \mathbf{s}(u_\alpha)) d\mathbf{s}(u_\alpha). \quad (25.19)$$

The polarization is in general time dependent, but in order to keep the notation brief the reference to time is here omitted. From now on we assume that all the curves are straight lines. For particle α this means that $\mathbf{s}(u_\alpha) = u\mathbf{r}_\alpha$, where $0 \leq u \leq 1$. As indicated, there is no need to put a subscript α on u from now on. The particular choice for the polarization field thus becomes

$$\mathbf{P}(\mathbf{r}) = \sum_\alpha \int_0^1 q_\alpha \mathbf{r}_\alpha \delta(\mathbf{r} - u\mathbf{r}_\alpha) du. \quad (25.20)$$

The presence of the Dirac delta function in (25.20) makes it easy to determine the polarization in reciprocal space. Hence,

$$\begin{aligned} P(q) &= \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \int_0^1 e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du \\ &= \sum_{\alpha} \frac{q_{\alpha} \mathbf{r}_{\alpha}}{i\mathbf{q} \cdot \mathbf{r}_{\alpha}} (1 - e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}}). \end{aligned} \quad (25.21)$$

We know from the analysis in Sect. 10.4.1 that the longitudinal part of the polarization, which in $\mathbf{q}$ -space is given by

$$\mathbf{P}_L(q) = \hat{\mathbf{q}} \hat{\mathbf{q}} \cdot \mathbf{P}(q) = \frac{\hat{\mathbf{q}}}{iq} \sum_{\alpha} q_{\alpha} (1 - e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}}), \quad (25.22)$$

is completely fixed by the charge density. To check this for the present choice of $\mathbf{P}(\mathbf{r})$, we transform the relation

$$i\mathbf{q} \cdot \mathbf{P}_L(q) = \sum_{\alpha} q_{\alpha} (1 - e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}}) \quad (25.23)$$

back to direct space. Here it reads

$$\nabla \cdot \mathbf{P}_L(\mathbf{r}) = \left(\sum_{\alpha} q_{\alpha} \right) \delta(\mathbf{r}) - \sum_{\alpha} q_{\alpha} \delta(\mathbf{r} - \mathbf{r}_{\alpha}). \quad (25.24)$$

For a globally neutral system one has

$$\sum_{\alpha} q_{\alpha} = 0, \quad (25.25)$$

and since the last term in (25.24) is precisely the charge density, we see that (10.44) is fulfilled. From a microscopic point of view only time dependent polarizations are of importance, cf. (10.41). This implies that even for systems which globally are not neutral, the first (static) term in (25.24) cannot play a physical role. In the absence of external charges we know that the nonstatic part of the electric displacement field is a transverse vector field; see (10.50).

25.2.2 Magnetization Field

Although it is possible to make a choice for the (time derivative of the) transverse polarization so that the generalized magnetization field vanishes identically, as we have realized in Sect. 10.4.1, the choice associated to the polarization field in (25.20)

must be accompanied by a magnetization field in order to represent the microscopic current density in (10.41) correctly. Below we shall calculate this magnetization field. It is convenient to carry out the various calculations in reciprocal space and then transform back to direct space. In the $\mathbf{q}$ -domain, (10.41) takes the form

$$i\mathbf{q} \times \mathbf{M}(\mathbf{q}) = \mathbf{J}(\mathbf{q}) - \frac{\partial}{\partial t} \mathbf{P}(\mathbf{q}), \quad (25.26)$$

leaving out as hitherto the reference to time. A calculation of the two terms on the right side of this equation allows us to identify the transverse magnetization field $\mathbf{M}_T(\mathbf{q}) = \mathbf{M}(\mathbf{q})$ for the choice $\mathbf{M}_L(\mathbf{q}) = 0$. The Fourier transform of the microscopic current density (2.29) is given by

$$\mathbf{J}(\mathbf{q}) = \sum_{\alpha} q_{\alpha} \dot{\mathbf{r}}_{\alpha} e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}}. \quad (25.27)$$

To obtain the time derivative of the polarization it is convenient to start from the integral expression given for $\mathbf{P}(\mathbf{q})$ in (25.21). Thus, one gets

$$\frac{\partial}{\partial t} \mathbf{P}(\mathbf{q}) = \sum_{\alpha} q_{\alpha} \dot{\mathbf{r}}_{\alpha} \int_0^1 e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du + \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} (-i\mathbf{q} \cdot \dot{\mathbf{r}}_{\alpha}) \int_0^1 u e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du. \quad (25.28)$$

If the first integral is integrated by parts one obtains next

$$\frac{\partial}{\partial t} \mathbf{P}(\mathbf{q}) = \sum_{\alpha} q_{\alpha} \dot{\mathbf{r}}_{\alpha} e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha}} + \sum_{\alpha} i q_{\alpha} (\dot{\mathbf{r}}_{\alpha} \mathbf{q} \cdot \mathbf{r}_{\alpha} - \mathbf{r}_{\alpha} \mathbf{q} \cdot \dot{\mathbf{r}}_{\alpha}) \int_0^1 u e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du. \quad (25.29)$$

Subtraction of the results in (25.27) and (25.29) then gives

$$\mathbf{J}(\mathbf{q}) - \frac{\partial}{\partial t} \mathbf{P}(\mathbf{q}) = i\mathbf{q} \times \left[\sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \times \dot{\mathbf{r}}_{\alpha} \int_0^1 u e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du \right], \quad (25.30)$$

as the reader readily may verify. By a comparison of (25.26) and (25.30) one finally is led to the following expression for the (transverse) magnetization in reciprocal space:

$$\mathbf{M}(\mathbf{q}) = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \times \dot{\mathbf{r}}_{\alpha} \int_0^1 u e^{-i\mathbf{q} \cdot \mathbf{r}_{\alpha} u} du, \quad (25.31)$$

so that in real space

$$\mathbf{M}(\mathbf{r}) = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \times \dot{\mathbf{r}}_{\alpha} \int_0^1 u \delta(\mathbf{r} - u\mathbf{r}_{\alpha}) du. \quad (25.32)$$

The specific choice given for the polarization in (25.20) thus must be accompanied by the magnetization in (25.32) in order to give, via (10.41), the physical microscopic current density in (2.29).

25.3 Lagrangians in the Coulomb and Poincaré Gauges

25.3.1 Nonrelativistic Standard Lagrangian and Its Gauge Transformation

The standard Lagrangian of classical electrodynamics is in the nonrelativistic limit given by

$$L^{\text{ST}} = L_{\text{P}}^{\text{ST}} + L_{\text{F}}^{\text{ST}} + L_{\text{I}}^{\text{ST}}, \quad (25.33)$$

where

$$L_{\text{P}}^{\text{ST}} = \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{\mathbf{r}}_{\alpha}^2(t) \quad (25.34)$$

is the Lagrangian for the particles (P),

$$L_{\text{F}}^{\text{ST}} = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} [\mathbf{E}^2(\mathbf{r}, t) - c_0^2 \mathbf{B}^2(\mathbf{r}, t)] d^3r \quad (25.35)$$

is the Lagrangian of the electromagnetic field (F), and

$$L_{\text{I}}^{\text{ST}} = \sum_{\alpha} q_{\alpha} [\dot{\mathbf{r}}_{\alpha}(t) \cdot \mathbf{A}(\mathbf{r}_{\alpha}, t) - \phi(\mathbf{r}_{\alpha}, t)] \quad (25.36)$$

is the interaction (I) Lagrangian. The Lagrangian above is (here) called the standard Lagrangian because it is the Lagrangian most often used in classical electrodynamics. For what follows it is convenient to specify this Lagrangian, and its various parts, by the superscript ST. The sum $L_{\text{P}}^{\text{ST}} + L_{\text{I}}^{\text{ST}}$ originates in the form the Lagrangian given by (11.77) and (11.78) takes in the nonrelativistic limit, leaving out an unnecessary constant rest mass energy term. In terms of the Lagrangian density

$$\mathcal{L}^{\text{ST}} = \frac{\epsilon_0}{2} [\mathbf{E}^2(\mathbf{r}, t) - c_0^2 \mathbf{B}^2(\mathbf{r}, t)] + \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{A}(\mathbf{r}, t) - \rho(\mathbf{r}, t)\phi(\mathbf{r}, t), \quad (25.37)$$

the standard Lagrangian can be written in the form

$$L^{\text{ST}} = L_{\text{P}}^{\text{ST}} + \int_{-\infty}^{\infty} \mathcal{L}^{\text{ST}}(\mathbf{r}, t) d^3r, \quad (25.38)$$

as the reader may verify using (2.28) and (2.29). Starting from (25.38), it is shown in many (advanced) textbooks (e.g., [178, 303]) that Lagrange's equations, for the particles and relative to the scalar and vector potential, lead to the Newton–Lorentz equations for the individual particles (2.30), and to the microscopic Maxwell–Lorentz equations which relate the fields to their sources ((2.2) and (2.3)). The source-free pair of Maxwell equations ((2.1) and (2.4)) results directly from the relations between $(\mathbf{E}, \mathbf{B})$ and $(\mathbf{A}, \phi)$ ((2.5) and (2.7)). In a sense, it is the recovering of the

microscopic Maxwell–Lorentz and Newton–Lorentz equations which a posteriori justifies the choice for the standard Lagrangian of classical electrodynamics.

The classical theory of electrodynamics is manifestly gauge invariant, although the standard Lagrangian does depend on the gauge choice. In L^{ST} it is however only the interaction part, L_I^{ST} , which is gauge dependent. The gauge transformation in (2.11) and (2.12) immediately shows that old (OLD) and new (NEW) standard interaction Lagrangians are related as follows:

$$(L_I^{\text{ST}})^{\text{NEW}} = (L_I^{\text{ST}})^{\text{OLD}} + \sum_{\alpha} q_{\alpha} \left(\dot{\mathbf{r}}_{\alpha}(t) \cdot \nabla \chi(\mathbf{r}_{\alpha}, t) + \frac{\partial}{\partial t} \chi(\mathbf{r}_{\alpha}, t) \right). \quad (25.39)$$

In compact form, (25.39) can be written

$$(L_I^{\text{ST}})^{\text{NEW}} = (L_I^{\text{ST}})^{\text{OLD}} + \frac{d}{dt} F(\{\mathbf{r}_{\alpha}\}, t), \quad (25.40)$$

where

$$F(\{\mathbf{r}_{\alpha}\}, t) = \sum_{\alpha} q_{\alpha} \chi(\mathbf{r}_{\alpha}, t). \quad (25.41)$$

The fact that the two Lagrangians deviate by a total derivative with respect to time of a function F which only depends on the particle coordinates, $\{\mathbf{r}_{\alpha}\}$, and on time makes it clear that all physical predictions following from either of these Lagrangians will be the same.

25.3.2 The Power–Zienau–Woolley Transformation

Let us now determine the explicit form of the function $F(\{\mathbf{r}_{\alpha}\}, t)$ in the Poincaré gauge. With the gauge function χ^{P} in (25.1) we obtain

$$F(\{\mathbf{r}_{\alpha}\}, t) = - \sum_{\alpha} \int_0^1 q_{\alpha} \mathbf{r}_{\alpha} \cdot \mathbf{A}_{\text{T}}(u \mathbf{r}_{\alpha}, t) du, \quad (25.42)$$

and by means of the identity

$$\mathbf{A}_{\text{T}}(u \mathbf{r}_{\alpha}, t) = \int_{-\infty}^{\infty} \delta(\mathbf{r} - u \mathbf{r}_{\alpha}) \mathbf{A}_{\text{T}}(\mathbf{r}, t) d^3 r, \quad (25.43)$$

F , upon interchange of integrations, can be written as follows

$$F(\{\mathbf{r}_{\alpha}\}, t) = - \int_{-\infty}^{\infty} \left[\sum_{\alpha} \int_0^1 q_{\alpha} \mathbf{r}_{\alpha} \delta(\mathbf{r} - u \mathbf{r}_{\alpha}) du \right] \cdot \mathbf{A}_{\text{T}}(\mathbf{r}, t) d^3 r. \quad (25.44)$$

Since the quantity in the square bracket is just the specific polarization introduced in Sect. 25.2.1 (25.20) we get

$$F(\{\mathbf{r}_\alpha\}, t) = - \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}, t) \cdot \mathbf{A}_T(\mathbf{r}, t) d^3r. \quad (25.45)$$

Despite the fact that we have come to the expression in (25.45) utilizing the Poincaré gauge in which the definition of the polarization refers to a single reference point, it is clear that the form in (25.45) can be used also for polarizations referring to several reference points. Such a generalization of the F in (25.45) is useful for instance in studies of the electrodynamic interaction between strongly localized systems of charges, e.g., atoms, molecules, and mesoscopic particles. With a multiplicity of reference points for the polarizations, the matching of the now generalized F in (25.45) to the Poincaré gauge is no longer possible. The transformation of the standard Lagrangian defined via (25.45), possibly generalized to a multiplicity of reference points for the polarization, is called the Power–Zienau–Woolley transformation [178, 318, 319]. Since only the transverse part of $\mathbf{P}$ contributes to the integral in (25.45), F can also be expressed in the form

$$F(\{\mathbf{r}_\alpha\}, t) = - \int_{-\infty}^{\infty} \mathbf{P}_T(\mathbf{r}, t) \cdot \mathbf{A}_T(\mathbf{r}, t) d^3r. \quad (25.46)$$

By means of the Parseval–Plancherel identity (9.56), the reader may readily express $-F$ as an integral of the scalar product $\mathbf{P}_T^*(\mathbf{q}; t)$ and $\mathbf{A}_T(\mathbf{q}; t)$ over the entire reciprocal space.

25.3.3 *On the Elimination of the Redundancy from the Standard Lagrangian*

We know from the analysis in Chap. 9 that the state of a global field–particle system is completely specified by giving at a given time (1) the transverse part of the electric field and the magnetic field at every space point, and (2) the positions and velocities of all particles. In describing the electromagnetic field by the potentials $\mathbf{A}$ and ϕ one has introduced an overabundance of degrees of freedom. All what is needed is the transverse part of the vector potential. As to the Lagrangian given by (25.34), (25.37), and (25.38) a more satisfactory physical situation thus is obtained by elimination of the scalar potential, ϕ , and the longitudinal part of the vector potential, $\mathbf{A}_L$.

The scalar potential appears via the integral

$$\int_{-\infty}^{\infty} \rho(\mathbf{r}, t) \phi(\mathbf{r}, t) d^3r = \int_{-\infty}^{\infty} \rho^*(\mathbf{q}; t) \phi(\mathbf{q}; t) \frac{d^3q}{(2\pi)^3}, \quad (25.47)$$

and in $\mathbf{q}$ -space the elimination of $\phi(\mathbf{q}; t)$ is easy because

$$\phi(\mathbf{q}; t) = \frac{1}{q^2} \left(\frac{1}{\epsilon_0} \rho(\mathbf{q}; t) + i \mathbf{q} \cdot \frac{\partial}{\partial t} \mathbf{A}_L(\mathbf{q}; t) \right), \quad (25.48)$$

as the reader may verify with the help of the Maxwell–Lorentz equation in (2.2), and (2.7). In principle, the scalar potential thus can be eliminated in favour of the particle position coordinates (entering ρ) and the longitudinal part of the vector potential. By inserting the expression for $\phi(\mathbf{q}; t)$ into (25.47) one obtains

$$\begin{aligned} \int_{-\infty}^{\infty} \rho(\mathbf{r}, t) \phi(\mathbf{r}, t) d^3 r &= \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} q^{-2} |\rho(\mathbf{q}; t)|^2 \frac{d^3 q}{(2\pi)^3} \\ &+ \int_{-\infty}^{\infty} i q^{-1} \rho^*(\mathbf{q}; t) \frac{\partial}{\partial t} A_L(\mathbf{q}; t) \frac{d^3 q}{(2\pi)^3}, \end{aligned} \quad (25.49)$$

with $A_L = \hat{\mathbf{q}} \cdot \mathbf{A}_L$. The longitudinal vector potential, which is a free variable, finally is eliminated by choosing the Coulomb gauge.

25.3.4 Coulomb Lagrangian: Regrouping of Parts

It appears from (9.59) and (9.60) that the first integral on the right side of (25.49) can be expressed in the form of a direct-space integral involving the longitudinal electric field, i.e.,

$$\epsilon_0^{-1} \int_{-\infty}^{\infty} q^{-2} |\rho(\mathbf{q}; t)|^2 \frac{d^3 q}{(2\pi)^3} = \epsilon_0 \int_{-\infty}^{\infty} E_L^2(\mathbf{r}, t) d^3 r. \quad (25.50)$$

From this result, and the decomposition $\mathbf{E}^2 = \mathbf{E}_T^2 + \mathbf{E}_L^2$, it follows that the Lagrangian density $\mathcal{L}^{\text{ST}}$ (25.37) in the Coulomb gauge, where it is denoted by $\mathcal{L}^{\text{C}}$, takes the simple form

$$\mathcal{L}^{\text{C}} = \frac{\epsilon_0}{2} [\mathbf{E}_T^2(\mathbf{r}, t) - c_0^2 \mathbf{B}^2(\mathbf{r}, t)] - \frac{\epsilon_0}{2} \mathbf{E}_L^2(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{A}_T(\mathbf{r}, t). \quad (25.51)$$

The integral of $(\epsilon_0/2) \mathbf{E}_L^2$ over the entire space is just the instantaneous Coulomb energy of the charge distribution, cf. (9.59) and (9.64). As we know, V_{Coul} can be expressed solely as a function of the particle position coordinates, see (9.68), and we therefore regroup it with the standard particle Lagrangian, L_p^{ST} , given in (25.34). The term in the sharp parenthesis in (25.51) (multiplied by $\epsilon_0/2$) is the Lagrangian density of the transverse electromagnetic field. All in all, we hence have obtained the following Coulomb Lagrangian:

$$L^{\text{C}} = L_p^{\text{C}} + L_F^{\text{C}} + L_I^{\text{C}}, \quad (25.52)$$

where

$$L_P^C = \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{\mathbf{r}}_{\alpha}^2(t) - \sum_{\alpha} \epsilon_{\text{self}}^{\alpha} - \frac{1}{8\pi\epsilon_0} \sum_{\alpha \neq \beta} \frac{q_{\alpha} q_{\beta}}{|\mathbf{r}_{\alpha}(t) - \mathbf{r}_{\beta}(t)|} \quad (25.53)$$

is the Lagrangian of the particles, and

$$L_F^C = \int_{-\infty}^{\infty} \mathcal{L}_F^C(\mathbf{r}, t) d^3r \quad (25.54)$$

is the Lagrangian of the transverse electromagnetic field, a part with a Lagrangian density

$$\mathcal{L}_F^C = \frac{\epsilon_0}{2} [E_T^2(\mathbf{r}, t) - c_0^2 \mathbf{B}^2(\mathbf{r}, t)] = \frac{\epsilon_0}{2} \left[\left(\frac{\partial}{\partial t} \mathbf{A}_T(\mathbf{r}, t) \right)^2 - c_0^2 (\nabla \times \mathbf{A}_T(\mathbf{r}, t))^2 \right]. \quad (25.55)$$

Finally,

$$L_I^C = \int_{-\infty}^{\infty} \mathcal{L}_I^C(\mathbf{r}, t) d^3r \quad (25.56)$$

is the interaction Lagrangian, which density is particularly simple, viz.,

$$\mathcal{L}_I^C = \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{A}_T(\mathbf{r}, t). \quad (25.57)$$

In a way, it is manifest that L^C is the Coulomb Lagrangian because only the transverse vector potential appears in the densities $\mathcal{L}_F^C$ and $\mathcal{L}_I^C$.

25.3.5 Poincaré Interaction Lagrangian

It is pretty clear from the analysis in Sects. 25.3.1 and 25.3.2 that the Poincaré (L^P) and Coulomb (L^C) Lagrangians are related as follows:

$$L^P = L^C + \frac{d}{dt} \left(- \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}, t) \cdot \mathbf{A}_T(\mathbf{r}, t) d^3r \right). \quad (25.58)$$

It is natural to group the dF/dt -term with the interaction Lagrangian, L_I^C . If this is done, both the particle and transverse field Lagrangians are identical in the two descriptions, of course. The Poincaré interaction Lagrangian, L_I^P , becomes

$$L_I^P = \int_{-\infty}^{\infty} (\mathbf{J} - \dot{\mathbf{P}}) \cdot \mathbf{A}_T d^3r - \int_{-\infty}^{\infty} \mathbf{P} \cdot \dot{\mathbf{A}}_T d^3r, \quad (25.59)$$

as one may realize by carrying out the d/dt -operation on the product under the integral sign in (25.58). The first integral in (25.59) can be rewritten by means of (10.41). Thus

$$\begin{aligned} \int_{-\infty}^{\infty} (\mathbf{J} - \dot{\mathbf{P}}) \cdot \mathbf{A}_T d^3r &= \int_{-\infty}^{\infty} (\nabla \times \mathbf{M}) \cdot \mathbf{A}_T d^3r \\ &= \int_{-\infty}^{\infty} \mathbf{M} \cdot \nabla \times \mathbf{A}_T d^3r. \end{aligned} \quad (25.60)$$

The last step in (25.60) is obtained using the identity $(\nabla \times \mathbf{M}) \cdot \mathbf{A}_T = \mathbf{M} \cdot \nabla \times \mathbf{A}_T + \nabla \cdot (\mathbf{M} \times \mathbf{A}_T)$. Upon integration over space, and subsequent use of Gauss theorem, it is seen that the contribution from the last term in this identity is zero. Since $\nabla \times \mathbf{A}_T = \mathbf{B}$ and $\dot{\mathbf{A}}_T = -\mathbf{E}_T$, we finally get

$$L_1^P = \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}, t) \cdot \mathbf{E}_T(\mathbf{r}, t) d^3r + \int_{-\infty}^{\infty} \mathbf{M}(\mathbf{r}, t) \cdot \mathbf{B}(\mathbf{r}, t) d^3r. \quad (25.61)$$

25.3.6 Multipole Interaction Lagrangian

If the transverse electromagnetic field is slowly varying in space across the domain where $\mathbf{P}$ and $\mathbf{M}$ are nonvanishing, it is often useful to expand to the $\mathbf{E}_T$ - and $\mathbf{B}$ -fields in a Taylor series around the reference point for the polarization, here the origin of the coordinate system. The Poincaré interaction Lagrangian then takes the form of a multipole expansion, viz.,

$$L_1^P = \mathbf{p}(t) \cdot \mathbf{E}_T(\mathbf{0}, t) + \mathbf{m}(t) \cdot \mathbf{B}(\mathbf{0}, t) + \mathbf{Q}(t) : \nabla \mathbf{E}_T(\mathbf{0}, t) + \cdots. \quad (25.62)$$

The electric ($\mathbf{p}$) and magnetic ($\mathbf{m}$) dipole moments, and the electric quadrupole moment ($\mathbf{Q}$) are easily calculated on the basis of (25.20) and (25.32). The calculation of $\mathbf{Q}$ proceeds as follows:

$$\begin{aligned} \mathbf{Q} &= \int_{-\infty}^{\infty} \mathbf{P} \mathbf{r} d^3r = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \int_0^1 \left[\int_{-\infty}^{\infty} \delta(\mathbf{r} - u \mathbf{r}_{\alpha}) \mathbf{r} d^3r \right] du \\ &= \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \mathbf{r}_{\alpha} \int_0^1 u du = \frac{1}{2} \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha} \mathbf{r}_{\alpha}. \end{aligned} \quad (25.63)$$

The expression thus obtained for the electric quadrupole moment tensor agrees with the one in (5.21). The reader may verify to himself that the expressions obtained for $\mathbf{p}$ and $\mathbf{m}$ are those given in (5.19) and (5.24).

25.4 Conjugate Momenta: Coulomb and Poincaré Hamiltonians

25.4.1 Conjugate Particle Momentum

For a particle–field system described by the Lagrangian L the momentum conjugate to the particle position variable $\mathbf{r}_\alpha$ is defined as the partial derivative of L with respect to the velocity $\dot{\mathbf{r}}_\alpha$. i.e.,

$$\mathbf{p}_\alpha \equiv \frac{\partial L}{\partial \dot{\mathbf{r}}_\alpha}, \quad (25.64)$$

in a notation where the i th coordinate of the momentum is given by $(\mathbf{p}_\alpha)_i = \partial L / \partial (\dot{\mathbf{r}}_\alpha)_i$. In the Poincaré Lagrangian the velocity $\dot{\mathbf{r}}_\alpha$ appears in the kinetic energy (25.53), and in the magnetic part of the interaction part ((25.61), with $\mathbf{M}$ given in (25.32)). By using the identity $\mathbf{r}_\alpha \times \dot{\mathbf{r}}_\alpha \cdot \mathbf{B} = -\dot{\mathbf{r}}_\alpha \cdot (\mathbf{r}_\alpha \times \mathbf{B})$ one obtains (keeping the time implicit in the notation)

$$\mathbf{p}_\alpha^P = m_\alpha \dot{\mathbf{r}}_\alpha - q_\alpha \mathbf{r}_\alpha \times \int_0^1 u \mathbf{B}(u \mathbf{r}_\alpha) du. \quad (25.65)$$

To remember that the calculation refers to the Poincaré gauge we have given the momentum a superscript P . Since the vector potential in the Poincaré gauge is given by (25.17) one may write (25.65) in the form

$$\mathbf{p}_\alpha^P = m_\alpha \dot{\mathbf{r}}_\alpha - q_\alpha \mathbf{A}^P(\mathbf{r}_\alpha). \quad (25.66)$$

In the Coulomb gauge, the interaction Lagrangian is given by (25.56) and (25.57), and here the velocity $\dot{\mathbf{r}}_\alpha$ appears in the microscopic current density; see (2.29). The particle momentum therefore becomes

$$\mathbf{p}_\alpha^C = m_\alpha \dot{\mathbf{r}}_\alpha - q_\alpha \mathbf{A}_T(\mathbf{r}_\alpha) \quad (25.67)$$

in this gauge (with superscript C for Coulomb). The reader might have anticipated the results in (25.66) and (25.67) since the kinetic particle momentum

$$m_\alpha \dot{\mathbf{r}}_\alpha = \mathbf{p}_\alpha^P - q_\alpha \mathbf{A}^P(\mathbf{r}_\alpha) = \mathbf{p}_\alpha^C - q_\alpha \mathbf{A}_T(\mathbf{r}_\alpha) \quad (25.68)$$

is a gauge invariant quantity, and $\mathbf{A}_T = \mathbf{A}^C$ is the total vector potential in the Coulomb gauge.

25.4.2 Conjugate Field Momentum

From the Lagrangian point of view the electromagnetic field is a system with a continuous ensemble of degrees of freedom. The dynamical position variable is the

vector potential $\mathbf{A}_T(\mathbf{r})$, $\mathbf{r}$ being here an index. In the continuous case the conjugate field momentum $\boldsymbol{\Pi}(\mathbf{r})$ associated with the variable $\mathbf{A}_T(\mathbf{r})$ is given by [178]

$$\boldsymbol{\Pi}(\mathbf{r}) \equiv \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{A}}_T(\mathbf{r})}, \quad (25.69)$$

where $\mathcal{L}$ is the Lagrangian density. In the Poincaré Lagrangian density, the vector $\dot{\mathbf{A}}_T = -\mathbf{E}_T$ appears in the field energy density (25.55), and in the interaction integrand $\mathbf{P}_T \cdot \mathbf{E}_T = -\mathbf{P}_T \cdot \dot{\mathbf{A}}_T$ (25.61). Since only the transverse part of the polarization contributes to the first integral in (25.61), as we already know (see (25.46)), one must use the form $\mathbf{P}_T \cdot \dot{\mathbf{A}}_T$, and *not* $\mathbf{P} \cdot \dot{\mathbf{A}}_T$ when calculating $\boldsymbol{\Pi}(\mathbf{r})$. In the Poincaré gauge, the conjugate field momentum with index $\mathbf{r}$ thus becomes

$$\boldsymbol{\Pi}^P(\mathbf{r}) = \epsilon_0 \dot{\mathbf{A}}_T(\mathbf{r}) - \mathbf{P}_T(\mathbf{r}) = -\epsilon_0 \mathbf{E}_T(\mathbf{r}) - \mathbf{P}_T(\mathbf{r}). \quad (25.70)$$

A comparison of (10.53) and (25.70) shows the remarkable result that the transverse part of the electric displacement field is just the negative of the conjugate field momentum, i.e.,

$$\boldsymbol{\Pi}^P(\mathbf{r}) = -\mathbf{D}_T(\mathbf{r}). \quad (25.71)$$

In the Coulomb gauge the vector $\dot{\mathbf{A}}_T(\mathbf{r})$ does not appear in the interaction Lagrangian, and the conjugate field momentum hence is just

$$\boldsymbol{\Pi}^C(\mathbf{r}) = \epsilon_0 \dot{\mathbf{A}}_T(\mathbf{r}) = -\epsilon_0 \mathbf{E}_T(\mathbf{r}) \quad (25.72)$$

in this gauge.

25.4.3 Hamiltonians

The Lagrangian, L , of the particle–field system is a function of the particle coordinates ($\{\mathbf{r}_\alpha\}$) and velocities ($\{\dot{\mathbf{r}}_\alpha\}$), and the field “coordinates” ($\mathbf{A}_T(\mathbf{r})$) and “velocities” ($\dot{\mathbf{A}}_T(\mathbf{r})$). The Hamiltonian, so important in classical and quantum electrodynamics, is defined by [178]

$$H = \sum_{\alpha} \dot{\mathbf{r}}_{\alpha} \cdot \mathbf{p}_{\alpha} + \int_{-\infty}^{\infty} \dot{\mathbf{A}}_T(\mathbf{r}) \cdot \boldsymbol{\Pi}(\mathbf{r}) d^3r - L, \quad (25.73)$$

and it is a function of the particle and field coordinates and the associated conjugate momenta.

To determine the Hamiltonian in the Poincaré gauge, H^P , we eliminate the velocities $\{\dot{\mathbf{r}}_\alpha\}$ and $\dot{\mathbf{A}}_T(\mathbf{r})$ by means of (25.66) and (25.70). I leave it to the reader to verify that the result one obtains is the following:

$$H^P = H_P^P + H_F^P + H_I^P, \quad (25.74)$$

where

$$H_P^P = \sum_{\alpha} \frac{1}{2m_{\alpha}} \left(\mathbf{p}_{\alpha}^P \right)^2 + V_{\text{coul}} + \frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_T^2(\mathbf{r}) d^3r \quad (25.75)$$

is the particle Hamiltonian,

$$H_F^P = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[\left(\frac{\boldsymbol{\Pi}^P(\mathbf{r})}{\epsilon_0} \right)^2 + c_0^2 (\nabla \times \mathbf{A}_T(\mathbf{r}))^2 \right] d^3r \quad (25.76)$$

is the field Hamiltonian, and

$$H_I^P = \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \boldsymbol{\Pi}^P(\mathbf{r}) \cdot \mathbf{P}_T(\mathbf{r}) d^3r + \sum_{\alpha} \frac{q_{\alpha}^2}{2m_{\alpha}} (A^P(\mathbf{r}_{\alpha}))^2 - \sum_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} \mathbf{p}_{\alpha}^P \cdot \mathbf{A}^P(\mathbf{r}_{\alpha}) \quad (25.77)$$

is the interaction Hamiltonian. Before commenting on the result above, it is useful to obtain the Hamiltonian in the Coulomb gauge. A straightforward calculation leads to

$$H^C = H_P^C + H_F^C + H_I^C, \quad (25.78)$$

where in the same notation as above, the three parts are given by

$$H_P^C = \sum_{\alpha} \frac{1}{2m_{\alpha}} (\mathbf{p}_{\alpha}^C)^2 + V_{\text{coul}}, \quad (25.79)$$

$$H_F^C = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[\left(\frac{\boldsymbol{\Pi}^C(\mathbf{r})}{\epsilon_0} \right)^2 + c_0^2 (\nabla \times \mathbf{A}_T(\mathbf{r}))^2 \right] d^3r, \quad (25.80)$$

and

$$H_I^C = \sum_{\alpha} \frac{q_{\alpha}^2}{2m_{\alpha}} (A_T(\mathbf{r}_{\alpha}))^2 - \sum_{\alpha} \frac{q_{\alpha}}{m_{\alpha}} \mathbf{p}_{\alpha}^C \cdot \mathbf{A}_T(\mathbf{r}_{\alpha}). \quad (25.81)$$

A comparison of (25.75) and (25.79) shows that Hamiltonian of the particles in the Poincaré gauge has an unfamiliar extra term proportional to the space integral of $\mathbf{P}_T^2$. The term only depends on the canonical position variables of the particles, and it appears as a correction to the Coulomb energy. The new term plays an interesting role in studies of the near-field interaction between two separated systems of charges. The structure of the field Hamiltonian is the same in the two gauges, see (25.76) and (25.80), but it must be bared in mind that the conjugate field momenta ((25.70) and (25.72)) relate in different manners to the transverse electric field. The interaction Hamiltonian in the Poincaré gauge (25.77) deviates from that in the Coulomb gauge (25.81) by a term which describes the interaction of the transverse polarization of the charge system with the transverse part of the electric displacement field. Since $\boldsymbol{\Pi}^P$ is a transverse vector field, one can replace $\mathbf{P}_T$ by $\mathbf{P}$ in the integral, i.e.,

$$\frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \boldsymbol{\Pi}^P(\mathbf{r}) \cdot \mathbf{P}_T(\mathbf{r}) d^3r = -\frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \mathbf{D}_T(\mathbf{r}) \cdot \mathbf{P}(\mathbf{r}) d^3r. \quad (25.82)$$

In the absence of external charges we know from the analysis in Sect. 10.4.2 that the generalized electric displacement is a purely transverse vector field, i.e., $\mathbf{D} = \mathbf{D}_T$. When $\mathbf{D}_L = \mathbf{0}$, one has from (10.49), $\epsilon_0 \mathbf{E}_L = -\mathbf{P}_L$. It is clear then that the Coulomb energy of the particle system is,

$$V_{\text{Coul}} = \frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_L^2(\mathbf{r}) d^3r. \quad (25.83)$$

Since $\mathbf{P}_L^2 + \mathbf{P}_T^2 = \mathbf{P}^2$, one ends up with the particularly simple expression

$$H_P^P = \sum_{\alpha} \frac{1}{2m_{\alpha}} \left(p_{\alpha}^P \right)^2 + \frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}^2(\mathbf{r}) d^3r \quad (25.84)$$

for the particle Hamiltonian in the Poincaré gauge.

25.5 Quantum Description in the Poincaré Gauge

25.5.1 Quantum Representations Related by a Unitary Transformation: A Brief Review

In quantum physics, unitary transformations play an important role. An operator $\hat{T}(t)$ is unitary provided

$$\hat{T}^{-1}(t) = \hat{T}^{\dagger}(t). \quad (25.85)$$

When applied to state vectors ($|\psi^{(1)}(t)\rangle$) and *observables* ($\hat{\mathcal{O}}^{(1)}(t)$) these change in accordance with

$$|\psi^{(2)}(t)\rangle = \hat{T}(t) |\psi^{(1)}(t)\rangle, \quad (25.86)$$

$$\hat{\mathcal{O}}^{(2)}(t) = \hat{T}(t) \hat{\mathcal{O}}^{(1)} \hat{T}^{\dagger}(t). \quad (25.87)$$

The relations in (25.86) and (25.87) furnish a change in representation from (1) to (2). The transformation in (25.87) ensures that all quantum mechanical mean values are identical in the two representations, as the following calculation shows:

$$\begin{aligned} \langle \psi^{(2)}(t) | \hat{\mathcal{O}}^{(2)}(t) | \psi^{(2)}(t) \rangle &= \langle \psi^{(1)}(t) | \hat{T}^{\dagger}(t) \hat{T}(t) \hat{\mathcal{O}}^{(1)}(t) \hat{T}^{\dagger}(t) \hat{T}(t) | \psi^{(1)}(t) \rangle \\ &= \langle \psi^{(1)}(t) | \hat{\mathcal{O}}^{(1)}(t) | \psi^{(1)}(t) \rangle. \end{aligned} \quad (25.88)$$

The invariance of the norm is obvious, because, if $\hat{\mathcal{O}}^{(1)}$ is the identity operator so will $\hat{\mathcal{O}}^{(2)}$ be.

The temporal evolutions in the two representations satisfy form-identical Schrödinger equations, viz.,

$$i\hbar \frac{d}{dt} | \psi^{(i)}(t) \rangle = \hat{H}^{(i)}(t) | \psi^{(i)}(t) \rangle, \quad i = 1, 2 \quad (25.89)$$

and the Hamiltonian operators are related via

$$\hat{H}^{(2)}(t) = \hat{T}(t) \hat{H}^{(1)}(t) \hat{T}^\dagger(t) + i\hbar \frac{d\hat{T}(t)}{dt} \hat{T}^\dagger(t). \quad (25.90)$$

To obtain the result in (25.90) one first takes the time derivative of each side of (25.89). Thereafter the Schrödinger equations in (25.89) are used, and finally the relation $| \psi^{(1)} \rangle = \hat{T}^\dagger | \psi^{(2)} \rangle$ is employed. The Hamilton operator has a special position in quantum physics due to the fact that it enters the description of the timely evolution of the state vector (25.89). It is therefore not surprising that the Hamilton operator only transforms in accordance with (25.87) if the unitary transformation has no explicit time dependence. The Schrödinger equation in (25.89) show that the state vector at an arbitrary instant t , $| \psi^{(i)}(t) \rangle$, is related to the state vector at an initial time t_0 , $| \psi^{(i)}(t_0) \rangle$, by

$$| \psi^{(i)}(t) \rangle = \hat{U}^{(i)}(t, t_0) | \psi^{(i)}(t_0) \rangle, \quad (25.91)$$

where $\hat{U}^{(i)}(t, t_0)$ is a linear operator, called the (time) evolution operator. In order to ensure that the transformation conserves the norm of the state vector, the $\hat{U}^{(i)}(t, t_0)$'s must be unitary, as the reader may prove to himself. If the Hamilton operator $\hat{H}^{(i)}$ is time-independent, the evolution operator exhibits translational invariance, i.e., $\hat{U}^{(i)}(t, t_0) = \hat{U}^{(i)}(t - t_0)$, cf. the analysis given of the evolution operator in the Schrödinger picture in Sect. 23.2.3. In order to determine the relation between the evolution operators in the two representations we proceed as follows:

$$\begin{aligned} | \psi^{(2)}(t) \rangle &= \hat{T}(t) | \psi^{(1)}(t) \rangle = \hat{T}(t) \hat{U}^{(1)}(t, t_0) | \psi^{(1)}(t_0) \rangle \\ &= \hat{T}(t) \hat{U}^{(1)}(t, t_0) \hat{T}^\dagger(t_0) | \psi^{(2)}(t_0) \rangle. \end{aligned} \quad (25.92)$$

Hence,

$$\hat{U}^{(2)}(t, t_0) = \hat{T}(t) \hat{U}^{(1)}(t, t_0) \hat{T}^\dagger(t_0). \quad (25.93)$$

The relation in (25.93) ensures that the probability amplitude that a system starting at t_0 in an initial state $| \phi_\alpha^{(i)}(t_0) \rangle$ ends up at t in a final state $| \phi_\beta^{(i)}(t) \rangle$ is the same in both representations. The proof is simple:

$$\begin{aligned} \langle \phi_\beta^{(2)}(t) | \hat{U}^{(2)}(t, t_0) | \phi_\alpha^{(2)}(t_0) \rangle &= \langle \phi_\beta^{(2)}(t) | \hat{T}(t) \hat{U}^{(1)}(t, t_0) \hat{T}^\dagger(t_0) | \phi_\alpha^{(2)}(t_0) \rangle \\ &= \langle \phi_\beta^{(1)}(t) | \hat{U}^{(1)}(t, t_0) | \phi_\alpha^{(1)}(t_0) \rangle. \end{aligned} \quad (25.94)$$

The last step follows easily by operating on (25.86) with $\hat{T}^\dagger(t)$. This gives in ket-space for $t = t_0$ $|\phi_\alpha^{(1)}(t_0)\rangle = \hat{T}^\dagger(t_0) |\phi_\alpha^{(2)}(t_0)\rangle$, and for $t = t$ in bra space $\langle \phi_\alpha^{(1)}(t) | = \langle \phi_\alpha^{(2)}(t) | \hat{T}(t)$. The result in (25.94) guarantees that all physical predictions will be the same in the two representations.

25.5.2 The Unitary Transformation Relating the Quantum Descriptions in the Coulomb and Poincaré Gauges

In order to bridge the gap between quantum electrodynamics in the Coulomb and Poincaré gauges, one makes the following choice for the unitary operator $\hat{T}$:

$$\hat{T} = \exp\left(\frac{i}{\hbar} \hat{F}\right), \quad (25.95)$$

where, inspired by (25.45),

$$\hat{F} = - \int_{-\infty}^{\infty} \hat{\mathbf{P}}(\mathbf{r}) \cdot \hat{\mathbf{A}}_T(\mathbf{r}) d^3r. \quad (25.96)$$

Although the operators in the integrand of (25.96) to begin with refer to the Coulomb gauge, we shall see that they are identical to the ones obtained upon transformation with $\hat{T}$ (25.87). The transverse vector potential operator thus is given by (23.47) and the polarization operator has the explicit integral form

$$\hat{\mathbf{P}}(\mathbf{r}) = \sum_{\alpha} q_{\alpha} \hat{\mathbf{r}}_{\alpha} \int_0^1 \delta(\mathbf{r} - u \hat{\mathbf{r}}_{\alpha}) du, \quad (25.97)$$

$\hat{\mathbf{r}}_{\alpha}$ being the position operator for particle α in the Coulomb gauge. Since $\hat{T}^{-1} = \exp(-i \hat{F}/\hbar)$, and $\hat{T}^\dagger = \exp(-i \hat{F}^\dagger/\hbar)$ the transformation in (25.95) is unitary only if $\hat{F} = \hat{F}^\dagger$. That the $\hat{F}$ -operator in (25.96) indeed is Hermitian follows from the fact that both $\hat{\mathbf{P}}(\mathbf{r})$ and $\hat{\mathbf{A}}_T(\mathbf{r})$ are manifestly Hermitian. By inserting (25.97) into (25.96) it appears that

$$\hat{F} = - \sum_{\alpha} q_{\alpha} \hat{\mathbf{r}}_{\alpha} \cdot \int_0^1 \hat{\mathbf{A}}_T(u \hat{\mathbf{r}}_{\alpha}) du = \sum_{\alpha} q_{\alpha} \hat{\chi}^P(\hat{\mathbf{r}}_{\alpha}), \quad (25.98)$$

where $\hat{\chi}^P(\hat{\mathbf{r}}_{\alpha})$ is the operator related to the gauge transformation which takes one from an initial gauge (here the Coulomb gauge) to the Poincaré gauge. The unitary transformation defined by (25.95) and (25.96), namely,

$$\hat{T} = \exp\left[\frac{i}{\hbar} \hat{F}(\{\hat{\mathbf{r}}_{\alpha}\}; \{\hat{\mathbf{A}}_T\})\right], \quad (25.99)$$

depends only on the generalized position operators of the particles ($\{\hat{\mathbf{r}}_\alpha\}$) and the transverse electromagnetic field ($\{\hat{\mathbf{A}}_T\}$). As we will soon see, this implies that all operators which depend only on the particle and/or field position operators in the initial representation will be the same in the new representation.

25.5.3 Transformation of Various Physical Quantities

As a consequence of the fundamental commutator relation

$$[\hat{\mathbf{r}}_\alpha, \hat{\mathbf{r}}_\beta] = \mathbf{0}, \quad (25.100)$$

already written down in (11.96), and the fact that the transformation in (25.99) does not depend on the particle momentum operators, the new (superscript NEW) particle position operators become identical with the initial ones, since $\hat{T}$ commutes with $\hat{\mathbf{r}}_\alpha$, i.e.,

$$\hat{\mathbf{r}}_\alpha^{\text{NEW}} = \hat{T} \hat{\mathbf{r}}_\alpha \hat{T}^\dagger = \hat{\mathbf{r}}_\alpha. \quad (25.101)$$

The new and original polarization operators are also identical, of course:

$$\hat{\mathbf{P}}^{\text{NEW}}(\mathbf{r}) = \hat{T} \hat{\mathbf{P}}(\mathbf{r}) \hat{T}^\dagger = \hat{\mathbf{P}}(\mathbf{r}). \quad (25.102)$$

The operator belonging to the longitudinal part of the electric field, viz.,

$$\hat{\mathbf{E}}_L(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_\alpha q_\alpha \frac{\mathbf{r} - \hat{\mathbf{r}}_\alpha}{|\mathbf{r} - \hat{\mathbf{r}}_\alpha|^3} \quad (25.103)$$

is not changed by the $\hat{T}$ -transformation, because it only depends on the particle position operators, i.e.,

$$\hat{\mathbf{E}}_L^{\text{NEW}}(\mathbf{r}) = \hat{T} \hat{\mathbf{E}}_L(\mathbf{r}) \hat{T}^\dagger = \hat{\mathbf{E}}_L(\mathbf{r}). \quad (25.104)$$

Let us now consider the transformation of the operators $\hat{\mathbf{A}}_T$, $\hat{\mathbf{B}}$ and $\hat{\mathbf{E}}_T$, which all are associated with the dynamics of the transverse part of the electromagnetic field. The transformation of $\hat{\mathbf{A}}_T$ and $\hat{\mathbf{B}}$ follows readily by use of the equal-time commutator relation

$$[\hat{\mathbf{A}}_T(\mathbf{r}, t), \hat{\mathbf{A}}_T(\mathbf{r}', t)] = \mathbf{0}. \quad (25.105)$$

It is easy to prove (25.105), and I leave this to the reader. Since the integrand of $\hat{F}$ in (25.96) depends only on $\hat{\mathbf{A}}_T$ it is clear that

$$\left[\hat{\mathbf{A}}_T(\mathbf{r}), \int_{-\infty}^{\infty} \hat{\mathbf{P}}(\mathbf{r}') \cdot \hat{\mathbf{A}}_T(\mathbf{r}') d^3 r' \right] = \mathbf{0}. \quad (25.106)$$

In turn this leads to

$$\hat{\mathbf{A}}_{\text{T}}^{\text{NEW}}(\mathbf{r}) = \hat{T} \hat{\mathbf{A}}_{\text{T}}(\mathbf{r}) \hat{T}^{\dagger} = \hat{\mathbf{A}}_{\text{T}}(\mathbf{r}), \quad (25.107)$$

and

$$\hat{\mathbf{B}}^{\text{NEW}}(\mathbf{r}) = \hat{T} \hat{\mathbf{B}}(\mathbf{r}) \hat{T}^{\dagger} = \hat{\mathbf{B}}(\mathbf{r}). \quad (25.108)$$

We have thus shown that the operators belonging to the transverse vector potential and the magnetic field are identical in the two representations.

As promised in the last remark in Sect. 25.5.2, we have now proved that the generalized position operators of the particle–field system are the same in the old and new representations; see (25.101) and (25.107).

We now turn the attention towards the transformation of the generalized momentum operators. For the particle momentum one has

$$\hat{\mathbf{p}}_{\alpha}^{\text{NEW}} = \hat{T} \hat{\mathbf{p}}_{\alpha} \hat{T}^{\dagger} = \hat{\mathbf{p}}_{\alpha} + \hat{T} \left(\hat{\mathbf{p}}_{\alpha} \hat{T}^{\dagger} \right). \quad (25.109)$$

To calculate $(\hat{\mathbf{p}}_{\alpha} \hat{T}^{\dagger})$ we use for $\hat{F}$ the last expression in (25.98). With $\partial/\partial \hat{\mathbf{r}}_{\alpha} \equiv \hat{\mathbf{V}}_{\alpha}$, we get

$$(\hat{\mathbf{p}}_{\alpha} \hat{T}^{\dagger}) = \frac{\hbar}{i} \hat{\mathbf{V}}_{\alpha} \exp \left(-\frac{i}{\hbar} \sum_{\alpha} q_{\alpha} \hat{\chi}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}) \right) = -q_{\alpha} \hat{T}^{\dagger} \hat{\mathbf{V}}_{\alpha} \hat{\chi}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}), \quad (25.110)$$

and from (25.14)

$$(\hat{\mathbf{p}}_{\alpha} \hat{T}^{\dagger}) = q_{\alpha} \hat{T}^{\dagger} \left(\hat{\mathbf{A}}_{\text{T}}(\hat{\mathbf{r}}_{\alpha}) - \hat{\mathbf{A}}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}) \right). \quad (25.111)$$

The new momentum operator for the particle α hence is given by

$$\hat{\mathbf{p}}_{\alpha}^{\text{NEW}} = \hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}) + q_{\alpha} \hat{\mathbf{A}}_{\text{T}}(\hat{\mathbf{r}}_{\alpha}). \quad (25.112)$$

The result in (25.112) is satisfactory because the mean value (in an arbitrary quantum state) of the kinematical momentum operator becomes identical in the two representations,

$$\begin{aligned} \langle \psi^{\text{NEW}} | \hat{\boldsymbol{\pi}}_{\alpha} | \psi^{\text{NEW}} \rangle &\equiv \langle \psi^{\text{NEW}} | \hat{\mathbf{p}}_{\alpha}^{\text{NEW}} - q_{\alpha} \hat{\mathbf{A}}_{\text{T}}^{\text{NEW}}(\hat{\mathbf{r}}_{\alpha}) | \psi^{\text{NEW}} \rangle \\ &= \langle \psi^{\text{NEW}} | \hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}) | \psi^{\text{NEW}} \rangle \\ &= \langle \psi | \hat{T}^{\dagger} \left(\hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}^{\text{P}}(\hat{\mathbf{r}}_{\alpha}) \right) \hat{T} | \psi \rangle \\ &= \langle \psi | \hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}_{\text{T}}(\hat{\mathbf{r}}_{\alpha}) | \psi \rangle \equiv \langle \psi | \hat{\boldsymbol{\pi}}_{\alpha} | \psi \rangle. \end{aligned} \quad (25.113)$$

To determine the transformation of the transverse field momentum operator, which in the Coulomb gauge is $\hat{\Pi}^C = -\epsilon_0 \hat{\mathbf{E}}_T$ (see (25.72)), we first transform $\hat{\mathbf{E}}_T$. The transverse electric field operator in the new representation, viz.,

$$\hat{\mathbf{E}}_T^{\text{NEW}} = \hat{T} \hat{\mathbf{E}}_T \hat{T}^\dagger = \exp\left(\frac{i}{\hbar} \hat{F}\right) \hat{\mathbf{E}}_T \exp\left(-\frac{i}{\hbar} \hat{F}\right) \quad (25.114)$$

is calculated by means of the so-called operator expansion theorem:

$$\exp(\hat{A}) \hat{B} \exp(-\hat{A}) = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \dots \quad (25.115)$$

The theorem can be proved easily by expanding the function $\hat{f}(x) \equiv \exp(x\hat{A})\hat{B}\exp(-x\hat{A})$ in a Taylor series (in x) about the origin. We have $\hat{f}'(0) = [\hat{A}, \hat{B}]$, $\hat{f}''(0) = [\hat{A}, [\hat{A}, \hat{B}]]$, etc., and by setting $x = 1$ by the end of the calculation, (25.115) follows. In the present case we thus need to calculate the commutator $[-\frac{i}{\hbar} \hat{F}, \hat{\mathbf{E}}_T]$. By means of the equal-time commutator between $\hat{\mathbf{A}}_T(\mathbf{r})$ and $\hat{\mathbf{E}}_T(\mathbf{r}')$, given in (24.34), it is not difficult to show that

$$\begin{aligned} \left[-\frac{i}{\hbar} \int_{-\infty}^{\infty} \hat{\mathbf{P}}(\mathbf{r}') \cdot \hat{\mathbf{A}}_T(\mathbf{r}') d^3 r', \hat{\mathbf{E}}_T(\mathbf{r}) \right] &= -\frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \hat{\mathbf{P}}(\mathbf{r}') d^3 r' \\ &= -\frac{1}{\epsilon_0} \hat{\mathbf{P}}_T(\mathbf{r}). \end{aligned} \quad (25.116)$$

From this result it appears that all the higher-order commutators vanish since $\hat{F}$ commutes with $\hat{\mathbf{P}}_T$. Altogether, we thus obtain

$$\hat{\mathbf{E}}_T^{\text{NEW}}(\mathbf{r}) = \hat{\mathbf{E}}_T(\mathbf{r}) - \epsilon_0^{-1} \hat{\mathbf{P}}_T(\mathbf{r}). \quad (25.117)$$

In the new (Poincaré) description the transverse part of the electric displacement operator, $\hat{\mathbf{D}}_T^{\text{NEW}}$, is given by

$$\hat{\mathbf{D}}_T^{\text{NEW}}(\mathbf{r}) = \epsilon_0 \hat{\mathbf{E}}_T^{\text{NEW}}(\mathbf{r}) + \hat{\mathbf{P}}_T^{\text{NEW}}(\mathbf{r}) = \epsilon_0 \hat{\mathbf{E}}_T(\mathbf{r}), \quad (25.118)$$

as the reader may verify using (25.102) and (25.117). In the absence of external fields we know that

$$\hat{\mathbf{E}}_L^{\text{NEW}}(\mathbf{r}) = -\epsilon_0^{-1} \hat{\mathbf{P}}_L^{\text{NEW}}(\mathbf{r}) \quad (25.119)$$

since both the longitudinal electric field and the longitudinal polarization are the same in the Coulomb and Poincaré gauges. In combination, (25.118) and (25.119) imply that

$$\hat{\mathbf{D}}^{\text{NEW}}(\mathbf{r}) = \epsilon_0 \hat{\mathbf{E}}_T(\mathbf{r}). \quad (25.120)$$

In the new representation the transverse field momentum operator

$$\hat{\Pi}^{\text{NEW}}(\mathbf{r}) = -\hat{\mathbf{D}}_T^{\text{NEW}}(\mathbf{r}) = -\epsilon_0 \hat{\mathbf{E}}_T(\mathbf{r}) \quad (25.121)$$

is the negative of the (transverse) electric displacement operator (in the new representation).

25.5.4 Canonical Quantization: Hamilton Operator

In the Poincaré representation, the conjugate position ($\hat{\mathbf{r}}_\alpha$) and momentum ($\hat{\mathbf{p}}_\alpha$) operators of the Coulomb representation are replaced by the operators ($\hat{\mathbf{r}}_\alpha^{\text{NEW}}$) (25.101) and ($\hat{\mathbf{p}}_\alpha^{\text{NEW}}$) (25.112). These new operators satisfy the fundamental commutator relations for the particles. The proof for this assertion proceeds as follows:

$$\begin{aligned} [\hat{\mathbf{r}}_\alpha^{\text{NEW}}, \hat{\mathbf{p}}_\alpha^{\text{NEW}}] &\equiv \hat{\mathbf{r}}_\alpha^{\text{NEW}} \hat{\mathbf{p}}_\beta^{\text{NEW}} - \hat{\mathbf{p}}_\beta^{\text{NEW}} \hat{\mathbf{r}}_\alpha^{\text{NEW}} \\ &= \hat{T} \hat{\mathbf{r}}_\alpha \hat{T}^\dagger \hat{T} \hat{\mathbf{p}}_\beta \hat{T}^\dagger - \hat{T} \hat{\mathbf{p}}_\beta \hat{T}^\dagger \hat{T} \hat{\mathbf{r}}_\alpha \hat{T}^\dagger \\ &= \hat{T} (\hat{\mathbf{r}}_\alpha \hat{\mathbf{p}}_\beta - \hat{\mathbf{p}}_\beta \hat{\mathbf{r}}_\alpha) \hat{T}^\dagger \equiv \hat{T} [\hat{\mathbf{r}}_\alpha, \hat{\mathbf{p}}_\beta] \hat{T}^\dagger. \end{aligned} \quad (25.122)$$

Since the commutator between $\hat{\mathbf{r}}_\alpha$ and $\hat{\mathbf{p}}_\beta$ is the c -number dyad $i\hbar\delta_{\alpha\beta}\mathbf{U}$, we obtain

$$[\hat{\mathbf{r}}_\alpha^{\text{NEW}}, \hat{\mathbf{p}}_\beta^{\text{NEW}}] = i\hbar\delta_{\alpha\beta}\mathbf{U}, \quad (25.123)$$

as claimed. In the new representation, the conjugate field position ($\hat{\mathbf{A}}_T(\mathbf{r})$) and momentum [$\hat{\mathbf{\Pi}}^C(\mathbf{r}) \equiv \mathbf{\Pi}(\mathbf{r})$] operators are replaced by new positions ($\hat{\mathbf{A}}_T^{\text{NEW}}(\mathbf{r})$) (25.107) and momentum ($\hat{\mathbf{\Pi}}^{\text{NEW}}(\mathbf{r})$) (25.121) operators. The new operators are the conjugate of each other, and satisfy as such the fundamental equal-time field commutator relation

$$[\hat{\mathbf{A}}_T^{\text{NEW}}(\mathbf{r}, t), \hat{\mathbf{\Pi}}^{\text{NEW}}(\mathbf{r}', t)] = i\hbar\delta_T(\mathbf{r} - \mathbf{r}'). \quad (25.124)$$

The proof for this claim runs parallel to the one given for the particle operators above, and rests on the fact that the fundamental field commutator in the Coulomb gauge (24.34) commutes with $\hat{T}$.

For what follows it is convenient to use for the mathematical operators in the Poincaré representation the same symbols as used in the Coulomb gauge. Hence, for the particles $\hat{\mathbf{r}}_\alpha^{\text{NEW}} \equiv \hat{\mathbf{r}}_\alpha (= \mathbf{r}_\alpha; \text{multiplication by } \mathbf{r}_\alpha)$, $\hat{\mathbf{p}}_\alpha^{\text{NEW}} \equiv \hat{\mathbf{p}}_\alpha = (\hbar/i)\nabla_\alpha$, and for the fields in the Schrödinger picture

$$\hat{\mathbf{A}}_T^{\text{NEW}} \equiv \hat{\mathbf{A}}_T(\mathbf{r}) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0\omega_q} \right)^{1/2} (\hat{a}_{qs}e^{i\mathbf{q}\cdot\mathbf{r}} + \hat{a}_{qs}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}}) \boldsymbol{\epsilon}_{qs}, \quad (25.125)$$

$$\hat{\mathbf{\Pi}}^{\text{NEW}} \equiv \hat{\mathbf{\Pi}}(\mathbf{r}) = -\epsilon_0 L^{-3/2} \sum_{q,s} i \left(\frac{\hbar\omega_q}{2\epsilon_0} \right)^{1/2} (\hat{a}_{qs}e^{i\mathbf{q}\cdot\mathbf{r}} - \hat{a}_{qs}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}}) \boldsymbol{\epsilon}_{qs}. \quad (25.126)$$

We end this chapter by giving the expressions for the various parts of the Hamilton operator in the Poincaré gauge,

$$\hat{H}^P = \hat{H}_P^P + \hat{H}_F^P + \hat{H}_I^P. \quad (25.127)$$

The particle part is

$$\hat{H}_P^P = \sum_{\alpha} \frac{1}{2m_{\alpha}} (\hat{\mathbf{p}}_{\alpha})^2 + \hat{V}_{\text{Coul}} + \frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \hat{\mathbf{P}}_T^2(\mathbf{r}) d^3r, \quad (25.128)$$

the field part is given by two equivalent expression, viz.,

$$\hat{H}_F^P = \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[\left(\frac{\hat{\mathbf{H}}(\mathbf{r})}{\epsilon_0} \right)^2 + c_0^2 (\nabla \times \hat{\mathbf{A}}_T(\mathbf{r}))^2 \right] d^3r = \sum_{q,s} \hbar \omega_q \left(\hat{a}_{qs}^{\dagger} \hat{a}_{qs} + \frac{1}{2} \right), \quad (25.129)$$

and the interaction part looks as follows:

$$\begin{aligned} \hat{H}_I^P = & \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \hat{\mathbf{H}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_T(\mathbf{r}) d^3r + \sum_{\alpha} \frac{q_{\alpha}^2}{2m_{\alpha}} \left(\hat{\mathbf{A}}^P(\hat{\mathbf{r}}_{\alpha}) \right)^2 \\ & - \sum_{\alpha} \frac{q_{\alpha}}{2m_{\alpha}} \left(\hat{\mathbf{p}}_{\alpha} \cdot \hat{\mathbf{A}}^P(\hat{\mathbf{r}}_{\alpha}) + \hat{\mathbf{A}}^P(\hat{\mathbf{r}}_{\alpha}) \cdot \hat{\mathbf{p}}_{\alpha} \right). \end{aligned} \quad (25.130)$$

In the last sum the scalar product of $\hat{\mathbf{p}}_{\alpha}$ and $\hat{\mathbf{A}}^P(\mathbf{r})$ has been correctly symmetrized due to the fact that the vector-potential operator in the Poincaré gauge, viz.,

$$\hat{\mathbf{A}}^P(\mathbf{r}) = - \int_0^1 u \hat{\mathbf{r}}_{\alpha} \times \hat{\mathbf{B}}(u \hat{\mathbf{r}}_{\alpha}) du, \quad (25.131)$$

is not transverse. The integral expression for $\hat{\mathbf{A}}^P(\hat{\mathbf{r}}_{\alpha})$ follows from (25.17).

Chapter 26

Photon-Field Operators: Wave-Packet Photons

In this chapter, we take up the central question of how to relate the quantum electrodynamic theory to photon wave mechanics as this is formulated in the energy wave function approach. Since the photon in the first-quantized description is related to the positive-frequency part of the electromagnetic field we start by dividing the transverse electric and magnetic free-field operators into their positive- and negative-frequency parts. In the plane-wave decomposition of the positive (negative)-frequency field part appears operators which annihilate (create) single quanta in the two helicity eigenstates. Two so-called free photon-field operators are then defined in analogy to the classical definition of the positive-frequency Riemann–Silberstein vectors. The bridge to photon wave mechanics is made by taking the matrix elements of these operators between a general one-photon state and the photon vacuum state. It is shown that the two matrix elements can be identified with the upper and lower components of the free-photon spinor. A single-photon state is always an eigenstate for the global photon number operator (with eigenvalue 1), but in general it is not an eigenstate of the global photon Hamilton operator, nor of the global photon momentum operator.

Instead of composing the photon-field operators from a linear superposition of plane-wave modes, one can construct them by superposition of wave-packet modes. A given classical wave packet (index i) is formed by superposition of plane waves (index j) with weight factors β_{ij} . If the β_{ij} -coefficients are chosen to be the elements of a unitary matrix $\{\beta_{ij}\}$, the set of wave packet modes forms a complete set, and the arbitrary free photon-field operator can then be expanded after this set. The expansion coefficients are operators which annihilate single light quanta in the various wave packets.

In the presence of field–matter interactions it is useful to introduce so-called matter-coupled photon-field operators. These are obtained from the free operators by replacing the various free-field annihilation operators, $\hat{a}_{qs}(0) \exp(-i\omega_q t)$, by the general ones, $\hat{a}_{qs}(t)$. Once field–matter interactions are in play, we know that it might be useful to work in the Poincaré gauge. After having established the form the set of Maxwell–Lorentz operator equations takes in this gauge, we introduce new matter-coupled photon-field operators based on the $\hat{\mathbf{D}}^{(+)}$ - and $\hat{\mathbf{B}}^{(+)}$ -operators. By the end of this chapter we answer the question: How does the photon state

during a spontaneous emission process link to the photon embryo concept in wave mechanics?

26.1 Free Photon-Field Operators

In wave mechanics, the photons are associated with the positive-frequency part of the electromagnetic field, the so-called analytical signal. In order to make the bridge between the second-quantized description and photon wave mechanics it is thus useful to decompose the various electromagnetic field operators into positive- and negative-frequency parts. Since we in this chapter aims at a quantum electrodynamic description based on an extension of the energy wave function formalism, the decomposition of the transverse electric and magnetic field operators is of particular importance. To begin with only free fields are considered. In the Heisenberg picture, one hence obtains from (23.43), (23.44), and (23.49), the following decomposition of the transverse electric field operator:

$$\hat{\mathbf{E}}_{\text{T}}(\mathbf{r}, t) = \hat{\mathbf{E}}_{\text{T}}^{(+)}(\mathbf{r}, t) + \hat{\mathbf{E}}_{\text{T}}^{(-)}(\mathbf{r}, t), \quad (26.1)$$

where

$$\hat{\mathbf{E}}_{\text{T}}^{(+)}(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0} \right)^{1/2} \hat{a}_{qs}(0) \boldsymbol{\epsilon}_{qs} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_q t)} \quad (26.2)$$

is the positive-frequency part of the operator, and

$$\hat{\mathbf{E}}_{\text{T}}^{(-)}(\mathbf{r}, t) = \left(\hat{\mathbf{E}}_{\text{T}}^{(+)}(\mathbf{r}, t) \right)^{\dagger} \quad (26.3)$$

its negative-frequency part. The analogous decomposition of the magnetic field operator, given in (23.48) in the Schrödinger picture, becomes

$$\hat{\mathbf{B}}(\mathbf{r}, t) = \hat{\mathbf{B}}^{(+)}(\mathbf{r}, t) + \hat{\mathbf{B}}^{(-)}(\mathbf{r}, t), \quad (26.4)$$

with

$$\begin{aligned} \hat{\mathbf{B}}^{(+)}(\mathbf{r}, t) &= \left(\hat{\mathbf{B}}^{(-)}(\mathbf{r}, t) \right)^{\dagger} \\ &= L^{-3/2} \sum_{q,s} i \left(\frac{\hbar \omega_q}{2\epsilon_0 c_0^2} \right)^{1/2} \hat{a}_{qs}(0) \boldsymbol{\kappa} \times \boldsymbol{\epsilon}_{qs} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_q t)}. \end{aligned} \quad (26.5)$$

Before proceeding the reader should note that the positive- and negative-frequency parts of the field operators contain only annihilation and creation operators, respectively.

In the equations above, the field polarization state associated to the individual $\mathbf{q}$ -modes has been expanded after orthogonal real unit vectors, satisfying (15.49)–(15.51). Let us now switch to a polarization state decomposition after helicity unit vectors, $\mathbf{e}_{q+}$ and $\mathbf{e}_{q-}$, and let us denote the related annihilation (creation) operators by $\hat{a}_{q+}$ ($\hat{a}_{q+}^\dagger$) and $\hat{a}_{q-}$ ($\hat{a}_{q-}^\dagger$). With the identification

$$\hat{a}_{q1}(0)\epsilon_{q1} + \hat{a}_{q2}(0)\epsilon_{q2} = \hat{a}_{q+}(0)\mathbf{e}_{q+} + \hat{a}_{q-}(0)\mathbf{e}_{q-}, \quad (26.6)$$

the positive frequency part of the electric field operator takes the form

$$\hat{\mathbf{E}}_T^{(+)}(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q}} i \left(\frac{\hbar\omega_{\mathbf{q}}}{2\epsilon_0} \right)^{1/2} (\hat{a}_{q+}(0)\mathbf{e}_{q+} + \hat{a}_{q-}(0)\mathbf{e}_{q-}) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)}. \quad (26.7)$$

The relations between the two sets of annihilation operators in (26.6) are (omitting for simplicity the reference to $\mathbf{q}$)

$$\hat{a}_+ = \frac{1}{\sqrt{2}}(\hat{a}_1 - i\hat{a}_2), \quad (26.8)$$

$$\hat{a}_- = \frac{1}{\sqrt{2}}e^{-i\delta}(-i\hat{a}_1 + \hat{a}_2), \quad (26.9)$$

as one may realize with the help of (15.53) and (15.54). The reader may verify, starting from (26.8) and (26.9), that the helicity operators satisfy the fundamental commutator relations in (23.41) and (23.42). To obtain the helicity-state expansion for the positive frequency part of the magnetic field operator, we multiply (26.6) vectorially with $\boldsymbol{\kappa}$ from the left, and use thereafter (15.72). The expression given for $\hat{\mathbf{B}}^{(+)}$ in (26.5) then becomes

$$\hat{\mathbf{B}}^{(+)}(\mathbf{r}, t) = L^{-3/2} \sum_{\mathbf{q}} \left(\frac{\hbar\omega_{\mathbf{q}}}{2\epsilon_0 c_0^2} \right)^{1/2} (\hat{a}_{q+}(0)\mathbf{e}_{q+} - \hat{a}_{q-}(0)\mathbf{e}_{q-}) e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)}. \quad (26.10)$$

One now defines two so-called free photon-field operators [213]

$$\hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(\hat{\mathbf{E}}_T^{(+)}(\mathbf{r}, t) \pm i c_0 \hat{\mathbf{B}}^{(+)}(\mathbf{r}, t) \right) \quad (26.11)$$

by analogy with the classical positive-frequency Riemann–Silberstein vectors (16.19). By insertion of (26.7) and (26.10) into (26.11) one obtains the following plane-wave expansions of the photon-field operators:

$$\hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, t) = i L^{-3/2} \sum_{\mathbf{q}} (\hbar\omega_{\mathbf{q}})^{1/2} \hat{a}_{q+}(0)\mathbf{e}_{q+} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)}, \quad (26.12)$$

$$\hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, t) = i L^{-3/2} \sum_{\mathbf{q}} (\hbar\omega_{\mathbf{q}})^{1/2} \hat{a}_{q-}(0)\mathbf{e}_{q-} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)}. \quad (26.13)$$

As the reader may have anticipated, the two field operators annihilate plane-wave quanta of positive ($\hat{\mathbf{F}}_+^{(+)}$) and negative ($\hat{\mathbf{F}}_-^{(+)}$) helicity.

26.2 Single-Photon States: Relation to Photon Wave Mechanics

To make contact to the wave mechanical description of the photon, let us now consider the general one-photon state

$$|\Phi\rangle = \left[L^{-3/2} \sum_{\mathbf{q}} \left(\alpha_{\mathbf{q}+} \hat{a}_{\mathbf{q}+}^{\dagger} + \alpha_{\mathbf{q}-} \hat{a}_{\mathbf{q}-}^{\dagger} \right) \right] |0\rangle, \quad (26.14)$$

where $|0\rangle$ is the global vacuum state of the field. For simplicity the fact that the operators are time independent is kept implicit in (26.14), and below, i.e., $\hat{a}_{\mathbf{q}+}^{\dagger}(0) = \hat{a}_{\mathbf{q}+}^{\dagger}$, etc. The bra-vector related to the ket-vector in (26.14) is

$$\langle\Phi| = \langle 0| \left[L^{-3/2} \sum_{\mathbf{q}} \left(\alpha_{\mathbf{q}+}^* \hat{a}_{\mathbf{q}+} + \alpha_{\mathbf{q}-}^* \hat{a}_{\mathbf{q}-} \right) \right]. \quad (26.15)$$

The states

$$|\Phi_{qs}\rangle \equiv \hat{a}_{qs}^{\dagger} |0\rangle, \quad s = +, -, \quad (26.16)$$

are single-photon states associated with plane waves of wave vector $\mathbf{q}$ and positive ($s = +$) and negative ($s = -$) helicity. The state $|\Phi\rangle$ is a linear superposition of such states over $\mathbf{q}$ and s . The one-photon state in (26.14) is normalized provided the otherwise arbitrary weight functions $\{\alpha_{qs}\}$ satisfy the condition

$$\langle\Phi|\Phi\rangle = L^{-3} \sum_{\mathbf{q}} (|\alpha_{\mathbf{q}+}|^2 + |\alpha_{\mathbf{q}-}|^2) = 1. \quad (26.17)$$

The first equality in (26.17) follows readily by use of the fundamental commutator relation in (23.42) (with $s, s' = +$ or $-$), as the reader may prove to herself. The c -number coefficients, $\{\alpha_{qs}\}$, in (26.14) are time independent since the probabilities for observing the photon in the various $(\mathbf{q}, s)$ -modes cannot be changed as a function of time for a free field.

The importance of the photon-field operators emerges when they act on the general single-photon state. For the positive-helicity operator one has

$$\hat{\mathbf{F}}_+^{(+)} |\Phi\rangle = i L^{-3} \sum_{\mathbf{q}, \mathbf{q}'} (\hbar \omega_{\mathbf{q}})^{1/2} \mathbf{e}_{\mathbf{q}+} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega_{\mathbf{q}} t)} \hat{a}_{\mathbf{q}+} \left(\alpha_{\mathbf{q}'+} \hat{a}_{\mathbf{q}'+}^{\dagger} + \alpha_{\mathbf{q}'-} \hat{a}_{\mathbf{q}'-}^{\dagger} \right) |0\rangle. \quad (26.18)$$

Since the annihilation and creation operators belonging to different $(\mathbf{q}, s)$ -modes commute (23.42), and $\hat{a}_{\mathbf{q}+} |0\rangle = 0$ for all $\mathbf{q}$, the double sum in (26.18) reduces to a

single sum. Hence,

$$\hat{\mathbf{F}}_+^{(+)}|\Phi\rangle = iL^{-3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q+} \mathbf{e}_{q+} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} \hat{a}_{q+} \hat{a}_{q+}^\dagger |0\rangle, \quad (26.19)$$

and finally

$$\hat{\mathbf{F}}_+^{(+)}|\Phi\rangle = iL^{-3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q+} \mathbf{e}_{q+} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} |0\rangle. \quad (26.20)$$

A similar calculation as the one above gives for the action of the negative-helicity operator on $|\Phi\rangle$ the result

$$\hat{\mathbf{F}}_-^{(+)}|\Phi\rangle = iL^{-3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q-} \mathbf{e}_{q-} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} |0\rangle. \quad (26.21)$$

The projections of the states in (26.20) and (26.21) onto the global vacuum state are

$$\begin{aligned} \langle 0 | \hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, t) | \Phi \rangle &= iL^{-3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q+} \mathbf{e}_{q+} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} \\ &\rightarrow \int_{-\infty}^{\infty} i (\hbar\omega_q)^{1/2} \alpha_+(q) \mathbf{e}_+(\kappa) e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} \frac{d^3q}{(2\pi)^3}, \end{aligned} \quad (26.22)$$

and

$$\begin{aligned} \langle 0 | \hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, t) | \Phi \rangle &= iL^{-3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q-} \mathbf{e}_{q-} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} \\ &\rightarrow \int_{-\infty}^{\infty} i (\hbar\omega_q)^{1/2} \alpha_-(q) \mathbf{e}_-(\kappa) e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_q t)} \frac{d^3q}{(2\pi)^3}, \end{aligned} \quad (26.23)$$

where the expression after the arrows are those obtained in the continuum limit. Remembering that $\omega_q = c_0 q$, a comparison to the plane-wave continuum superposition of the photon wave functions $f_\pm^{(+)}$ ((16.39) with (16.41) inserted) shows that the identifications

$$f_\pm^{(+)}(q) = i (\hbar\omega_q)^{1/2} \alpha_\pm(q) \quad (26.24)$$

allow one to recover the photon energy wave functions via the projections in (26.22) and (26.23). The factor i in (26.24) is not essential, since it can be included as an overall phase shift of the helicity unit vectors. Starting from the second-quantized theory, the spinorial free-photon energy wave function of the first-quantized formalism (16.26) thus is reproduced as

$$\Phi(\mathbf{r}, t) = \begin{pmatrix} \langle 0 | \hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, t) | \Phi \rangle \\ \langle 0 | \hat{\mathbf{F}}_-^{(-)}(\mathbf{r}, t) | \Phi \rangle \end{pmatrix}. \quad (26.25)$$

26.3 Local and Global Bilinear Operators: Nonstationary One-Photon States

From the vectorial photon-field operators we now form two bilinear scalar operators, viz.,

$$\hat{\mathbf{F}}_{\pm}^{(-)}(\mathbf{r}, t) \cdot \hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t) = \left(\hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t) \right)^{\dagger} \cdot \hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t). \quad (26.26)$$

These operators are local and Hermitian, and their mean values in the one-photon state $|\Phi\rangle$ (26.14) follow immediately from (26.20) and (26.21). Thus,

$$\begin{aligned} \langle \Phi | \left(\hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) \right)^{\dagger} \cdot \hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) | \Phi \rangle \\ = L^{-6} \sum_{\mathbf{q}, \mathbf{q}'} \hbar(\omega_{\mathbf{q}}\omega_{\mathbf{q}'})^{1/2} \alpha_{\mathbf{q}'s}^* \alpha_{\mathbf{q}s} \mathbf{e}_{\mathbf{q}'s}^* \cdot \mathbf{e}_{\mathbf{q}s} e^{i[(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r} - (\omega_{\mathbf{q}} - \omega_{\mathbf{q}'}t)]} \\ = \left(\mathbf{f}_s^{(+)}(\mathbf{r}, t) \right)^* \cdot \mathbf{f}_s^{(+)}(\mathbf{r}, t), \quad s = +, -. \end{aligned} \quad (26.27)$$

The last member of (26.27) follows from (26.24), and the discrete plane-wave superposition of the one-photon Riemann–Silberstein vectors

$$\mathbf{f}_s^{(+)}(\mathbf{r}, t) = L^{-3} \sum_{\mathbf{q}} \mathbf{f}_s^{(+)}(\mathbf{q}) \mathbf{e}_{\mathbf{q}s} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega_{\mathbf{q}}t)}, \quad (26.28)$$

cf. (16.39). The quantum mechanical mean values in (26.27) hence equal the local one-photon energy density in the two helicity states. One must here emphasize once again the limited physical meaning of the field energy density concept in *both* photon physics and classical electrodynamics.

The Hamilton operator of the free photon field ($\hat{H}_{\text{PH}}$) is obtained by integrating the bilinear operators in (26.26) over the entire space (quantization volume, V) and adding up thereafter the contributions from the two helicities. Thus,

$$\begin{aligned} \hat{H}_{\text{PH}} \equiv \hat{H}_{\text{F}} - \frac{1}{2} \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} &= \sum_{s=+,-} \int_V \left(\hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) \right)^{\dagger} \cdot \hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) d^3r \\ &= \sum_{\mathbf{q}, s} \hbar\omega_{\mathbf{q}} \hat{a}_{\mathbf{q}s}^{\dagger} \hat{a}_{\mathbf{q}s}. \end{aligned} \quad (26.29)$$

The integrand in (26.29) contains a double sum, over say $\mathbf{q}$ and $\mathbf{q}'$, and its $\mathbf{r}$ -dependence is of the form $\exp[i(\mathbf{q} - \mathbf{q}') \cdot \mathbf{r}]$. The integration over V , thus results in the appearance of the Kronecker delta $\delta_{\mathbf{q}, \mathbf{q}'}$, and this fact reduces the double sum

to a single sum over $\mathbf{q}$. This sum is nothing more than the one given in the last member of (26.29). The reader may prove to himself that the global momentum operator of the free photon field is given by

$$\begin{aligned} \mathbf{P}_F &= (ic_0)^{-1} \sum_{s=+,-} \int_V \left(\hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) \right)^\dagger \times \hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) d^3r \\ &= \sum_{\mathbf{q}, s} \hbar \mathbf{q} \hat{a}_{\mathbf{q}s}^\dagger \hat{a}_{\mathbf{q}s}. \end{aligned} \quad (26.30)$$

The results in (26.29) and (26.30) agree with the findings of Sect. 23.1.5.

The one-photon state in (26.14) is in general *not* an eigenstate of $\hat{H}_{\text{PH}}$, nor of $\mathbf{P}_F$. The action of $\hat{H}_{\text{PH}}$ on $|\Phi\rangle$ thus gives

$$\hat{H}_{\text{PH}}|\Phi\rangle = L^{-3/2} \sum_{\mathbf{q}, s} \hbar \omega_{\mathbf{q}} \alpha_{\mathbf{q}s} \hat{a}_{\mathbf{q}s}^\dagger |0\rangle. \quad (26.31)$$

Unless the superposition is over $\mathbf{q}$ -modes having the same magnitude, the right-hand-side of (26.31) is not proportional to $|\Phi\rangle$. The single-photon eigenstate $|\Phi\rangle$ is therefore in general not a stationary photon state.

The space-time propagation of the energy in a nonstationary one-photon state is particularly simple in the case where the superposition in (26.14) only contains $\mathbf{q}$ -modes in a given direction, say $\boldsymbol{\kappa}$. The photon energy density in a given helicity state ($s = +, -$), i.e.,

$$\left| \hat{\mathbf{F}}_s^{(+)}(\mathbf{r}, t) |\Phi\rangle \right|^2 = \left| L^{-3} \sum_{\mathbf{q}} (\hbar \omega_{\mathbf{q}})^{1/2} \alpha_{\mathbf{q}s} e^{i\mathbf{q} \cdot (\boldsymbol{\kappa} \cdot \mathbf{r} - c_0 t)} \right|^2, \quad (26.32)$$

thus propagates without distortion, and with the vacuum speed of light, in the $\boldsymbol{\kappa}$ -direction.

In finishing this section it should be mentioned that the bilinear operator $\sum_s (\hat{\mathbf{F}}_s^{(+)})^\dagger \cdot \hat{\mathbf{F}}_s^{(+)}$ plays an important role in the theory of a photoelectric light detection [53, 348].

26.4 Wave-Packet Photon Operators and States

The modes we have been considering so far are plane waves of definite wave vector $\mathbf{q}$ and definite polarization s , and by linear superposition of such modes we have introduced photon-field operators $\hat{\mathbf{F}}_+^{(+)}$ and $\hat{\mathbf{F}}_-^{(+)}$ for the two helicity species, and general single-photon states, $|\Phi\rangle$. Instead of plane-wave modes one can use wave packets of different forms as a basis for the representation of the electromagnetic field, and its related operators and quantum states. With reference to the quantized Riemann–Silberstein formalism for photons, we shall in the following briefly discuss one particular approach to the wave packet description.

As a starting point we consider classical wave packets formed by linear combinations of plane-wave modes, viz.,

$$\mathbf{u}_i(\mathbf{r}, t) = L^{-3/2} \sum_j \beta_{ij} \mathcal{F}_j \mathbf{e}_j e^{i(\mathbf{q}_j \cdot \mathbf{r} - \omega_j t)}. \quad (26.33)$$

The various wave packets $\mathbf{u}_i(\mathbf{r}, t)$ are identified by the subscript i , and the actual plane-wave superposition appearing in a given wave packet is determined by the β_{ij} -coefficients. A plane-wave mode is identified by the set $(\mathbf{q}, s)$, and in (26.33) and below a single index, say j , designates the set. The factor

$$\mathcal{F}_j \equiv i(\hbar\omega_j)^{1/2} \quad (26.34)$$

is the same as the one appearing in the expansions of the photon-field operators; see (26.12) and (26.13). For reasons to be given below, it is convenient to separate out this factor in (26.33). The β_{ij} -coefficients are now chosen to be the elements of a unitary matrix $\boldsymbol{\beta}$, i.e.,

$$\boldsymbol{\beta}^{-1} = \boldsymbol{\beta}^\dagger. \quad (26.35)$$

The definition in (26.35) is tantamount to the requirement

$$\sum_i \beta_{ij}^* \beta_{ik} = \delta_{jk}. \quad (26.36)$$

The choice in (26.35) allows one to express the generalized photon-field operator

$$\hat{\mathbf{F}}^{(\dagger)}(\mathbf{r}, t) \equiv \sum_{s=+,-} \hat{\mathbf{F}}_s^{(\dagger)}(\mathbf{r}, t) \quad (26.37)$$

in an interesting compact form, as we shall see now. With the help of the Kronecker delta the operator first is written as a double sum, viz.,

$$\begin{aligned} \hat{\mathbf{F}}^{(+)}(\mathbf{r}, t) &= L^{-3/2} \sum_k \mathcal{F}_k \hat{a}_k(0) \mathbf{e}_k e^{i(\mathbf{q}_k \cdot \mathbf{r} - \omega_k t)} \\ &= L^{-3/2} \sum_{j,k} \delta_{jk} \hat{a}_j(0) \mathcal{F}_k \mathbf{e}_k e^{i(\mathbf{q}_k \cdot \mathbf{r} - \omega_k t)}. \end{aligned} \quad (26.38)$$

Thereafter, the unitarity criterion in (26.36) is used to rewrite the expression for $\hat{\mathbf{F}}^{(+)}$ as follows:

$$\begin{aligned} \hat{\mathbf{F}}^{(+)}(\mathbf{r}, t) &= L^{-3/2} \sum_{i,j,k} \beta_{ij}^* \beta_{ik} \hat{a}_j(0) \mathcal{F}_k \mathbf{e}_k e^{i(\mathbf{q}_k \cdot \mathbf{r} - \omega_k t)} \\ &= \sum_{i,j} \beta_{ij}^* \hat{a}_j(0) \mathbf{u}_i(\mathbf{r}, t). \end{aligned} \quad (26.39)$$

A new time independent $\hat{c}_i(0)$, defined by the linear combination of annihilation operators,

$$\hat{c}_i(0) \equiv \sum_j \beta_{ij}^* \hat{a}_j(0), \quad (26.40)$$

finally allows one to write the generalized free photon-field operator in the important form

$$\hat{\mathbf{F}}^{(+)}(\mathbf{r}, t) = \sum_i \hat{c}_i(0) \mathbf{u}_i(\mathbf{r}, t). \quad (26.41)$$

It appears plausible from (26.41) that the $\hat{c}_i(0)$'s play the role of annihilation operators for light quanta belonging to the wave-packet modes defined by the $\mathbf{u}_i$'s in (26.33). To verify this, it is necessary that the $\hat{c}_i(0)$ -operators, and their Hermitian conjugates $\hat{c}_i^\dagger(0)$, satisfy the fundamental commutator relations for boson annihilation and creation operators. It follows at once from (23.41) that

$$[\hat{c}_i(0), \hat{c}_j(0)] = [\hat{c}_i^\dagger(0), \hat{c}_j^\dagger(0)] = 0, \quad (26.42)$$

and on the basis of (23.42) and (26.36) one obtains

$$\begin{aligned} [\hat{c}_i(0), \hat{c}_j^\dagger(0)] &= \sum_{k,l} \beta_{ik}^* \beta_{jl} [\hat{a}_k(0), \hat{a}_l^\dagger(0)] \\ &= \sum_{k,l} \beta_{ik}^* \beta_{jl} \delta_{kl} = \sum_k \beta_{ik}^* \beta_{jk} \\ &= \sum_k \beta_{kj}^* \beta_{ki} = \delta_{ij}. \end{aligned} \quad (26.43)$$

Hence, it has been shown that the fundamental commutation relations indeed are satisfied.

In Sect. 26.2 general one-photon states were built by linear superposition of single-photon plane-wave states. Single-photon wave packets may also be superimposed to form more general one-photon states. The state

$$|\Phi\rangle = \left[L^{-3/2} \sum_j \alpha_j \hat{c}_j^\dagger \right] |0\rangle, \quad (26.44)$$

thus represents a normalized single-photon state provided

$$\begin{aligned} \langle \Phi | \Phi \rangle &= \langle 0 | L^{-3} \sum_{i,j} \alpha_j^* \alpha_i \hat{c}_j \hat{c}_i^\dagger | 0 \rangle \\ &= \langle 0 | L^{-3} \sum_i |\alpha_i|^2 (\hat{c}_i^\dagger \hat{c}_i + 1) | 0 \rangle \\ &= L^{-3} \sum_i |\alpha_i|^2 = 1. \end{aligned} \quad (26.45)$$

The bridge from the state in (26.44) to photon wave mechanics is made by forming the matrix element of the photon-field operator in (26.41) between the global vacuum state and the one-photon state in (26.44). An elementary calculation readily gives

$$\langle 0 | \hat{\mathbf{F}}^{(+)}(\mathbf{r}, t) | \Phi \rangle = L^{-3} \sum_i \alpha_i \mathbf{u}_i(\mathbf{r}, t), \quad (26.46)$$

and the right-hand-side of this equation is just the expected superposition of classical wave packets of the form given in (26.33).

The wave-packet mode functions in (26.33) are not mutually orthogonal as the following calculation shows:

$$\begin{aligned} \int_V \mathbf{u}_i^*(\mathbf{r}, t) \cdot \mathbf{u}_j(\mathbf{r}, t) d^3r &= L^{-3} \sum_{k,l} \beta_{ik}^* \beta_{jl} \mathcal{F}_k^* \mathcal{F}_l \mathbf{e}_k^* \cdot \mathbf{e}_l e^{i(\omega_k - \omega_l)t} \int_V e^{i(\mathbf{q}_l - \mathbf{q}_k) \cdot \mathbf{r}} d^3r \\ &= \sum_{k,l} \beta_{ik}^* \beta_{jl} \mathcal{F}_k^* \mathcal{F}_l \mathbf{e}_k^* \cdot \mathbf{e}_l e^{i(\omega_k - \omega_l)t} \delta_{kl} \\ &= \sum_k |\mathcal{F}_k|^2 \beta_{ik}^* \beta_{jk} = \sum_k \hbar \omega_k \beta_{ik}^* \beta_{jk}. \end{aligned} \quad (26.47)$$

It is the presence of the $\mathcal{F}_j$ -factors in (26.33) which prevents the modes from being orthogonal. In the present context it is fruitful to include these $\mathcal{F}_j$'s in the definition of the mode functions because the same coefficients enter the expression for the photon-field operator $\hat{\mathbf{F}}^{(+)}(\mathbf{r}, t)$; see (26.38). In studies where other operators appear it is in general not so useful to include the $\mathcal{F}_j$'s in the mode function definition. By leaving out the $\mathcal{F}_j$ -coefficients from the expansion in (26.33) it appears from (26.36) and (26.47) that the new mode functions form an orthonormal set. The reader may show to himself that the new set is also complete. Any field operator could be expanded in terms of the new set of mode functions. Without the presence of the $\mathcal{F}_j$'s, the resulting annihilation and creation operators do not satisfy commutation relations as simple as those in (26.42) and (26.43).

26.5 Maxwell–Lorentz Operator Equations in the Poincaré Gauge

It was shown in Chap. 22 that the set of Maxwell–Lorentz operator equations in the Coulomb gauge has the following form:

$$\nabla \times \hat{\mathbf{E}}_T(\mathbf{r}, t) = -\frac{\partial}{\partial t} \hat{\mathbf{B}}(\mathbf{r}, t), \quad (26.48)$$

$$\nabla \times \hat{\mathbf{B}}(\mathbf{r}, t) = \mu_0 \hat{\mathbf{J}}_T(\mathbf{r}, t) + \frac{1}{c_0^2} \frac{\partial}{\partial t} \hat{\mathbf{E}}_T(\mathbf{r}, t), \quad (26.49)$$

$$\nabla \cdot \hat{\mathbf{E}}_L(\mathbf{r}, t) = \frac{1}{\epsilon_0} \hat{\rho}(\mathbf{r}, t), \quad (26.50)$$

$$\nabla \cdot \hat{\mathbf{B}}(\mathbf{r}, t) = 0, \quad (26.51)$$

in a notation where the T–L structure of the various vector fields has been emphasized. The Maxwell operator equations above are form-identical to the classical Maxwell–Lorentz equations. In the Coulomb gauge the dynamical field variables are $\mathbf{A}_T$ and $-\epsilon_0 \mathbf{E}_T$, and the Maxwell operator equations in (26.48) and (26.49) give the connection between the corresponding operators, remembering that $\mathbf{B} = \nabla \times \mathbf{A}_T$.

In the Poincaré gauge the dynamical field variables are $\mathbf{A}_T$ and $-\mathbf{D}_T (= -\mathbf{D})$, and in this gauge the Maxwell operator equations express the connection between the related operators. Instead of $\hat{\mathbf{J}}_T$ and $\hat{\rho}$, the particle operators $\nabla \times \hat{\mathbf{P}}_T$ and $\nabla \times \hat{\mathbf{M}}$ now enter. The two inhomogeneous operator equations may be obtained from the Heisenberg equation of motions for $\hat{\mathbf{B}}^{\text{NEW}} = \hat{\mathbf{B}}$ and $\epsilon_0 \hat{\mathbf{E}}_T^{\text{NEW}} = \hat{\mathbf{D}}$ using the Poincaré Hamilton operator, given in (25.127)–(25.130). Alternatively, the transformation formula $\hat{\mathbf{E}}_T = \epsilon_0^{-1}(\hat{\mathbf{D}} - \hat{\mathbf{P}}_T)$ and $\hat{\mathbf{J}}_T = \partial \hat{\mathbf{P}}_T / \partial t + \nabla \times \hat{\mathbf{M}}$ can be used to eliminate the old operators $\hat{\mathbf{E}}_T$ and $\hat{\mathbf{J}}_T$ in (26.48) and (26.49) in favour of the new ones. The operators $\hat{\mathbf{P}}_T$ and $\hat{\mathbf{M}}$ are identical in the Coulomb and Poincaré gauges since they only depend on the particle position coordinates, as we have already explicitly stressed for the polarization operator in (25.102). The operator equation in (26.50) transforms into a dynamical equation which expresses the transversality of the $\hat{\mathbf{D}}$ -operator, as the reader may prove to himself. Altogether, it appears that the Maxwell–Lorentz operator equations in the Poincaré gauge are as follows:

$$\nabla \times \hat{\mathbf{D}}(\mathbf{r}, t) = \nabla \times \hat{\mathbf{P}}_T(\mathbf{r}, t) - \epsilon_0 \frac{\partial}{\partial t} \hat{\mathbf{B}}(\mathbf{r}, t), \quad (26.52)$$

$$\nabla \times \hat{\mathbf{B}}(\mathbf{r}, t) = \mu_0 \nabla \times \hat{\mathbf{M}}(\mathbf{r}, t) + \mu_0 \frac{\partial}{\partial t} \hat{\mathbf{D}}(\mathbf{r}, t), \quad (26.53)$$

$$\nabla \cdot \hat{\mathbf{D}}(\mathbf{r}, t) = 0, \quad (26.54)$$

$$\nabla \cdot \hat{\mathbf{B}}(\mathbf{r}, t) = 0. \quad (26.55)$$

It is not surprising that this set of operator relations is form-identical to the set of classical Maxwell–Lorentz equations, when these are expressed in terms of $\mathbf{D}$, $\mathbf{B}$, $\mathbf{P}_T$ and $\mathbf{M}$.

26.6 Matter-Coupled Photon-Field Operators

In the presence of field–matter interaction the annihilation operator $\hat{a}_{qs}$ satisfies the dynamical equation in (23.137). The complete solution of this first-order differential equation is given by

$$\hat{a}_{qs}(t) = \hat{a}_{qs}(0)e^{-i\omega_q t} + i(2\epsilon_0\hbar\omega_q)^{-1/2}e^{-i\omega_q t} \int_{-\infty}^t \epsilon_{qs} \cdot \hat{\mathbf{J}}(\mathbf{q}; t') e^{i\omega_q t'} dt'. \quad (26.56)$$

The first term on the right-hand-side of this equation describes the free evolution of the annihilation operator, and the second term accounts for the modification brought about by the field-matter coupling in the time evolution. The polarization index s in (26.56) may classify the helicity states [$\epsilon_{qs} = \mathbf{e}_{qs}$, $s = +, -$]. With the replacements $\hat{a}_{q+}(0) \exp(-i\omega_q t) \Rightarrow \hat{a}_{q+}(t)$ and $\hat{a}_{q-}(0) \exp(-i\omega_q t) \Rightarrow \hat{a}_{q-}(t)$ in the expressions for the field operators in (26.7) and (26.10) two generalized photon-field operators are defined via (26.11). The plane-wave expansions of the generalized operators have the following forms:

$$\hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, t) = iL^{-3/2} \sum_q (\hbar\omega_q)^{1/2} \hat{a}_{q+}(t) \mathbf{e}_{q+} e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (26.57)$$

$$\hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, t) = iL^{-3/2} \sum_q (\hbar\omega_q)^{1/2} \hat{a}_{q-}(t) \mathbf{e}_{q-} e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (26.58)$$

In the Poincaré gauge it is convenient to introduce new matter-coupled photon-field operators by the definitions

$$\hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t) = \sqrt{\frac{\epsilon_0}{2}} \left(\epsilon_0^{-1} \hat{\mathbf{D}}^{(+)}(\mathbf{r}, t) \pm i c_0 \hat{\mathbf{B}}^{(+)}(\mathbf{r}, t) \right). \quad (26.59)$$

The *mathematical* operators representing the photon-field operators in the Poincaré gauge are the same as those in the Coulomb gauge, i.e., in the plane-wave decomposition the expressions given in (26.57) and (26.58).

26.7 Photon Embryo in Spontaneous Emission

The photon-field operator concept offers an elegant manner of establishing contact not only to the free photon energy wave function, as we have shown in Sect. 26.2, but also to the photon embryo formalism. To illustrate this let us consider the time dependent superposition

$$|\Psi(t)\rangle = L^{-3/2} \sum_{q,s=+,-} \alpha_{qs}(t) \hat{a}_{qs}^{\dagger}(0) |0\rangle. \quad (26.60)$$

The state vector represents a coherent superposition of one-photon helicity states which changes in time because the various α_{qs} -coefficients depend on t . Since we *do not* require that these coefficients satisfy the normalization condition in (26.17), $|\Psi(t)\rangle$ is not a genuine single-photon state. A superposition of the form given in (26.60), with a time-dependent norm

$$\langle \Psi(t) | \Psi(t) \rangle = L^{-3} \sum_{q,s} |\alpha_{qs}(t)|^2, \quad (26.61)$$

appears for instance *during* the spontaneous emission of a photon from an atom, a process we shall consider briefly in the next chapter. The state vector in (26.60) is given in the Schrödinger picture. In this picture, the photon-field operators are $\hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, 0)$ and $\hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, 0)$. For the picture-invariant matrix elements of these operators between the states $|0\rangle$ and $|\Psi(t)\rangle$ one obtains the results

$$\langle 0 | \hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, 0) | \Psi(t) \rangle = \frac{i}{L^3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q+}(t) \mathbf{e}_{q+} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad (26.62)$$

$$\langle 0 | \hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, 0) | \Psi(t) \rangle = \frac{i}{L^3} \sum_q (\hbar\omega_q)^{1/2} \alpha_{q-}(t) \mathbf{e}_{q-} e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (26.63)$$

We know from our studies of the photon embryo concept in Chap. 18 that the Riemann–Silberstein energy wave function embryo in direct space are described via the functions

$$\mathbf{f}_\pm^{(+)}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{f}_\pm^{(+)}(\mathbf{q}; t) \mathbf{e}_\pm(\kappa) e^{i\mathbf{q}\cdot\mathbf{r}} \frac{d^3q}{(2\pi)^3}. \quad (26.64)$$

If one goes to the continuum limit in (26.62) and (26.63), and then makes the identifications

$$\mathbf{f}_\pm^{(+)}(\mathbf{q}; t) = i(\hbar\omega_q)^{1/2} \alpha_\pm(\mathbf{q}; t), \quad (26.65)$$

it becomes clear that the photon embryo spinor is given by [180]

$$\boldsymbol{\Psi}(\mathbf{r}, t) = \begin{pmatrix} \langle 0 | \hat{\mathbf{F}}_+^{(+)}(\mathbf{r}, 0) | \Psi(t) \rangle \\ \langle 0 | \hat{\mathbf{F}}_-^{(+)}(\mathbf{r}, 0) | \Psi(t) \rangle \end{pmatrix}. \quad (26.66)$$

When the spontaneous emission process has been completed (rigorously speaking in the limit $t \rightarrow \infty$), the photon has been released from the atom with certainty. The energy wave function of the now free photon is given by

$$\lim_{t \rightarrow \infty} \boldsymbol{\Psi}(\mathbf{r}, t) = \boldsymbol{\Phi}(\mathbf{r}, t), \quad (26.67)$$

where $\boldsymbol{\Phi}(\mathbf{r}, t)$ is the spinorial state in (26.25).

Chapter 27

Photon Emission From Atoms: Elements of the Nonrelativistic QED Description

We begin this chapter with a brief introduction to the theory of spontaneous emission, and we add some remarks on the Lamb shift. For mesoscopic (and microscopic) objects, the field retardation across the transverse current density domain of the source usually will be small. The Lamb shift can be determined without the inclusion of retardation effects, but a calculation of the spontaneous emission requires that the field retardation is taken into account. That the spontaneous emission process depends on retardation is already clear from Einstein's phenomenological approach, where it turns out that the time rate of spontaneous emission (given by the well known Einstein A-coefficient [301, 324]) is proportional to c_0^{-3} . For $c_0 \rightarrow \infty$, $A \rightarrow 0$. For electric dipole-allowed transitions the spontaneous decay rate of the electron can be obtained including retardation to first order, only. It is indicated that there exists a close link between the field driving the spontaneous emission and the electric radiation reaction field studied in a classical framework in Chap. 17. After having studied the propagator connection between the photon-field operators and the polarization and magnetization field operators of the source, we turn our attention towards the field radiation from single-particle sources. Via a second-quantization of the source current density the important flip operators are introduced. In a somewhat sketchy manner we determine the classical electric-dipole Hamiltonian starting from the Poincaré Hamiltonian. The associated Hamilton operator we obtain by means of a rigorous so-called long-wavelength unitary transformation of the Coulomb Hamiltonian. In order to illustrate some of the basic aspects of the field-atom interaction we analyze in some detail the electrodynamics of so-called two-level atoms. We set up Heisenberg equations of motions for the atomic flip operator and the annihilation operator of the various field modes, and with these coupled dynamical equations in hand, and on the basis of certain approximations, we calculate the rate of spontaneous emission. We also briefly discuss the Lamb shift parameter, and the somewhat complicated physics we need to address in order to obtain an accurate value for it. In the last part of the chapter, we study the radiated transverse field, and we demonstrate that the spontaneous decay rate can be expressed in terms of the imaginary part of the transverse field propagator evaluated for coincident source and observation points.

27.1 Integral Relations Between Field and Particle Operators

27.1.1 On the Nonrelativistic Lamb Shift and Spontaneous Emission

Our purpose here is not to undertake a detailed study of these two fundamental electrodynamic phenomena but just to accentuate the fact that they are intimately linked. We shall return to the quantum electrodynamic theory for the spontaneous emission process later in this chapter.

We begin our discussion from the following integral relation between the transverse vector potential ($\hat{A}_T$) and current density ($\hat{J}_T$) operators:

$$\hat{A}_T(\mathbf{r}, t) = \hat{A}_T^{\text{ext}}(\mathbf{r}, t) + \mu_0 \int_{-\infty}^{\infty} g(R, \tau) \hat{J}_T(\mathbf{r}', t') dt' d^3 r', \quad (27.1)$$

where, in the usual notation, $R = |\mathbf{r} - \mathbf{r}'|$ and $\tau = t - t'$. The integral relation in (27.1) is exact and can be derived from the Maxwell operator equations given in Sect. 26.5. Since the transverse part of the vector potential (operator) is gauge invariant calculations carried out in respectively the Coulomb and Poincaré (or in any other gauge) lead to the same result, of course. It is also important that (27.1) can be established by a synthesis of the transverse vector-potential operator in the Heisenberg picture from the dynamical integral equations for the various photon annihilation (creation) operators. For the present purpose it is useful to carry out the integration over time in (17.1). Hence, one obtains

$$\hat{A}_T(\mathbf{r}, t) = \hat{A}_T^{\text{ext}}(\mathbf{r}, t) + \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} |\mathbf{r} - \mathbf{r}'|^{-1} \hat{J}_T\left(\mathbf{r}', t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0}\right) d^3 r', \quad (27.2)$$

a still exact relation. Let us assume now that the photon source is an atom or a mesoscopic particle. In these cases it is usually correct to say that the retardation time between any pair of points ($\mathbf{r}, \mathbf{r}'$) located within the transverse current density domain will be small in comparison to the characteristic time for variations in the electronic current density. For observation points in the rim zone (or inside our particle) it is thus useful to expand $\hat{J}_T(\mathbf{r}', t - R/c_0)$ in a Taylor series around $\hat{J}_T(\mathbf{r}', t)$. By keeping only the first two terms in the series, (27.2) is reduced to

$$\hat{A}_T(\mathbf{r}, t) = \hat{A}_T^{\text{ext}}(\mathbf{r}, t) + \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\hat{J}_T(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3 r' - \frac{\mu_0}{4\pi c_0} \frac{d}{dt} \int_{-\infty}^{\infty} \hat{J}_T(\mathbf{r}', t) d^3 r'. \quad (27.3)$$

As we shall realize soon, it turns out that the term

$$\hat{A}_T^{\text{Lamb}}(\mathbf{r}, t) \equiv \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\hat{J}_T(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \quad (27.4)$$

is responsible for the fact that the electromagnetic field radiated from a given (atomic) quantum transition is not centered on the electronic transition frequency, but is displaced slightly from it. The frequency shift is called the Lamb shift. Evidence for this shift was first provided by Lamb and Retherford in 1947 [325], who measured a frequency shift of the order 10^3 MHz for the atomic $2p_{1/2} \rightarrow 2s_{1/2}$ transition in hydrogen. In the same year, Bethe [327] calculated the Lamb shift for this transition to be ≈ 1.040 MHz. It appears from (27.4) that the Lamb shift survives in the nonretarded ($c_0 \rightarrow \infty$) limit, and the presence of the denominator $|\mathbf{r} - \mathbf{r}'|$ indicates that the shift depends on the detailed electronic structure of the source. From an optical near-field perspective the effect is quite interesting because the integration in (27.4) necessarily involves the entire rim zone of the source.

The last term of (27.3),

$$\hat{A}_T^{\text{spont}}(t) \equiv -\frac{\mu_0}{4\pi c_0} \frac{d}{dt} \int_{-\infty}^{\infty} \hat{\mathbf{J}}_T(\mathbf{r}, t) d^3r, \quad (27.5)$$

is responsible for the fact that for instance an atom in an excited state decays “spontaneously” towards its ground state. The effect is characteristic of a quantum field since it appears in the vacuum state of the external photon field and is independent of the photon occupation number. In the spontaneous decay process a photon is emitted from the source. Two important features of the spontaneous emission immediately appear from (27.5): (1) The process requires that the field retardation is taken into account (c_0 finite), and (2) the effect does not depend on the structure of the electronic current density since only the space integral of $\hat{\mathbf{J}}_T$ appears. As it stands, (27.5) involves an integration over the entire near-field zone of the mesoscopic (microscopic) source, but by making use of the result

$$\int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') d^3r' = \frac{2}{3} U, \quad (27.6)$$

it follows upon interchange of the $\mathbf{r}$ - and $\mathbf{r}'$ -integrations that

$$\int_{-\infty}^{\infty} \hat{\mathbf{J}}_T(\mathbf{r}, t) d^3r = \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \hat{\mathbf{J}}(\mathbf{r}', t) d^3r' d^3r = \frac{2}{3} \int_{-\infty}^{\infty} \hat{\mathbf{J}}(\mathbf{r}', t) d^3r'. \quad (27.7)$$

The spontaneous decay process hence depends on the integral of the current density (operator) over the source domain. One may prove (27.6) as follows: Start from (9.19), and integrate the last term first. This immediately gives $(2/3)U$. The first term is given as an integral over reciprocal space, and then integrated. Thus, in view of (9.13), one obtains (with $\kappa = \mathbf{q}/q$)

$$(2\pi)^{-3} \int_{-\infty}^{\infty} (U - \kappa\kappa) e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} d^3q d^3r = \int_{-\infty}^{\infty} (U - \kappa\kappa) \delta(\mathbf{q}) d^3q = \mathbf{0}. \quad (27.8)$$

That the last $\mathbf{q}$ -integral vanishes is readily seen by writing down the integral in spherical coordinates. This concludes the proof.

There is a deep connection between spontaneous emission and radiation reaction. A glimpse of this appears if one in the formula for the spontaneous emission operator

$$\hat{A}_T^{\text{spon}}(t) = -\frac{\mu_0}{6\pi c_0} \frac{d}{dt} \int_{-\infty}^{\infty} \hat{\mathbf{J}}(\mathbf{r}, t) d^3r \quad (27.9)$$

inserts the expression given in (23.132) for the current density operator $\hat{\mathbf{J}}(\mathbf{r}, t)$, evaluated in the Heisenberg picture. The occurrence of the delta function $\delta(\mathbf{r} - \mathbf{r}_\alpha)$ enables us to carry out the integration, and hence get

$$\hat{A}_T^{\text{spon}}(t) = -\frac{\mu_0}{6\pi c_0} \frac{d^2}{dt^2} \left(\sum_{\alpha} q_{\alpha} \hat{\mathbf{r}}_{\alpha}(t) \right) \quad (27.10)$$

since $\hat{\mathbf{v}}_{\alpha} = d\hat{\mathbf{r}}_{\alpha}/dt$. The quantity

$$\hat{\mathbf{p}}(t) = \sum_{\alpha} q_{\alpha} \hat{\mathbf{r}}_{\alpha}(t) \quad (27.11)$$

is the operator associated with the electric dipole moment of the source, cf. (5.19). For the electric field operator related to $\hat{A}_T^{\text{spon}}$, we thus obtain

$$\hat{\mathbf{E}}_T^{\text{spon}}(t) = \frac{1}{6\pi\epsilon_0 c_0^3} \frac{d^3}{dt^3} \hat{\mathbf{p}}(t). \quad (27.12)$$

By a comparison of this expression to the formula for the electric radiation reaction field for a single particle (7.29), it appears that (27.12) can be interpreted as the radiation reaction operator associated with the assembly of particles in the source. In the semiclassical (field unquantized) approach, also called the self-field approach, which has been extensively investigated over the years [360–366] it is predicted that an atom will decay “spontaneously” as a result of the interaction of the atom with its own self-field. The result in (27.12) leads in the direction of this alternative view of the physics behind spontaneous field emission. The two alternative explanations for the spontaneous decay viz., (1) interaction of the electron with its own field and (2) vacuum fluctuations in the quantum field, can be identified in a more elaborate QED calculation, see [328].

27.1.2 Propagator Connection Between the Photon-Field and Source-Particle Operators

Let us now return to the set of Maxwell operator equations as it appears in the Poincaré gauge ((26.52)–(26.55)). From these equations one may obtain the following inhomogeneous wave equations for the electric displacement and magnetic field operators:

$$\square \hat{\mathbf{D}}(\mathbf{r}, t) = \nabla \times \left(c_0^{-2} \frac{\partial}{\partial t} \hat{\mathbf{M}}(\mathbf{r}, t) - \nabla \times \hat{\mathbf{P}}(\mathbf{r}, t) \right) \quad (27.13)$$

and

$$\square \hat{\mathbf{B}}(\mathbf{r}, t) = -\mu_0 \nabla \times \left(\frac{\partial}{\partial t} \hat{\mathbf{P}}(\mathbf{r}, t) + \nabla \times \hat{\mathbf{M}}(\mathbf{r}, t) \right). \quad (27.14)$$

Since the magnetic field operator is the same in the Coulomb and Poincaré gauges, (27.14) is also identical in these gauges. This agrees with the fact that the quantity in the parenthesis is just the current density operator $\hat{\mathbf{J}}(\mathbf{r}, t)$ (cf. (10.41)), a gauge invariant vector field operator. The particular solutions to the equations above, namely,

$$\hat{\mathbf{D}}(\mathbf{r}, t) = \int_{-\infty}^{\infty} g(R, \tau) \nabla' \times \left(\nabla' \times \hat{\mathbf{P}}(\mathbf{r}', t') - c_0^{-2} \frac{\partial}{\partial t'} \hat{\mathbf{M}}(\mathbf{r}', t') \right) d^3 r' d\tau', \quad (27.15)$$

and

$$\hat{\mathbf{B}}(\mathbf{r}, t) = \mu_0 \int_{-\infty}^{\infty} g(R, \tau) \nabla' \times \left(\frac{\partial}{\partial t'} \hat{\mathbf{P}}(\mathbf{r}', t') + \nabla' \times \hat{\mathbf{M}}(\mathbf{r}', t') \right) d^3 r' d\tau', \quad (27.16)$$

describe in the Heisenberg picture the primary field operators $\hat{\mathbf{D}}/\epsilon_0$ and $\hat{\mathbf{B}}$ generated by what here is considered to be the sources of these fields. The source for the magnetic field is of course the same in the Coulomb and Poincaré gauges, but the source of $\hat{\mathbf{D}}(\mathbf{r}, t)$ (Poincaré gauge) and $\hat{\mathbf{E}}_T(\mathbf{r}, t)$ (Coulomb gauge) are not identical. Since, the source dependent part of $\hat{\mathbf{E}}_T$ is given by

$$\hat{\mathbf{E}}_T(\mathbf{r}, t) = -\mu_0 \int_{-\infty}^{\infty} g(R, \tau) \frac{\partial}{\partial t'} \hat{\mathbf{J}}_T(\mathbf{r}', t') d^3 r' d\tau', \quad (27.17)$$

the source region for $\hat{\mathbf{E}}_T$ extends over the entire near-field zone of the source particles, as we already have realized in the field-unquantized approach. The source region of the $\hat{\mathbf{D}}$ -field, on the other hand, is truncated to the electronic size of the mesoscopic (atomic) particle. The price one has to pay for this is that two vector fields, $\hat{\mathbf{P}}$ and $\hat{\mathbf{M}}$, are needed in the Poincaré gauge, but only one, $\hat{\mathbf{J}}_T$, in the Coulomb gauge. In both gauges the primary fields ($\hat{\mathbf{E}}_T$ and $\hat{\mathbf{B}}$) are transverse vector fields, and, as the presence of the Huygens propagator shows, these are always retarded outside their respective source regions. In the context of near-field electrodynamics, this implies that there is no instantaneous interaction between two mesoscopic particles (or atoms) in near-field contact in the Poincaré description. The reason for this originates in the fact that the $\hat{\mathbf{D}}$ - and $\hat{\mathbf{E}}_T$ -operators are related by a transformation

$$\hat{\mathbf{D}}(\mathbf{r}, t) = \epsilon_0 \hat{\mathbf{E}}_T(\mathbf{r}, t) + \nabla \times \int_{-\infty}^{\infty} \frac{\nabla' \times \hat{\mathbf{P}}(\mathbf{r}', t)}{4\pi |\mathbf{r} - \mathbf{r}'|} d^3 r', \quad (27.18)$$

which, although local in time, is nonlocal in space as far as the polarization operator is concerned. It is this nonlocality, which extends over the rim zone, that removes the instantaneous matter–field coupling of the Coulomb gauge.

In Sect. 26.6, matter-coupled photon-field operators for the Poincaré gauge were introduced by the definitions in the equations in (26.59). These operators consist of free-field parts, denoted by $\hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t; \text{FREE})$, and parts describing the radiation emission from the source. On the basis of the analytical parts of (27.15) and (27.16), the reader may verify that the photon-field operators of the two helicity species are given by

$$\begin{aligned} \hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t) = & \hat{\mathbf{F}}_{\pm}^{(+)}(\mathbf{r}, t; \text{FREE}) + (2\epsilon_0)^{-1} \int_{-\infty}^{\infty} g(R, \tau) \nabla' \\ & \times \left[\left(\pm \frac{i}{c_0} \frac{\partial}{\partial t'} + \nabla' \times \right) \left(\hat{\mathbf{P}}^{(+)}(\mathbf{r}', t') \pm \frac{i}{c_0} \hat{\mathbf{M}}^{(+)}(\mathbf{r}', t') \right) \right] d^3 r' dt'. \end{aligned} \quad (27.19)$$

It appears from this equation that the particle operators only appear in the combinations $\hat{\mathbf{P}}^{(+)} \pm i c_0^{-1} \hat{\mathbf{M}}^{(+)}$. The related classical combinations is the analytical part of

$$\mathbf{P} \pm \frac{i}{c_0} \mathbf{M} = \sum_{\alpha} q_{\alpha} \int_0^1 \left(\mathbf{r}_{\alpha} \pm \frac{i}{c_0} u \mathbf{r}_{\alpha} \times \dot{\mathbf{r}}_{\alpha} \right) \delta(\mathbf{r} - u \mathbf{r}_{\alpha}) du. \quad (27.20)$$

It follows from (27.20) that the ratio between the magnetization and polarization contributions is of the order v_{α}/c_0 .

27.2 Field Radiation from Single-Particle Source

27.2.1 Second-Quantization of Source Current Density: Flip Operators

Let us now assume that our source contains just one electro-dynamically active particle (electron, say), and that the particle spin plays no role. In the context of (27.1), a particle appears spinless in cases where the contribution from the spin current density to $\mathbf{J}_T$ is negligible. For both microscopic (atomic, molecular) and mesoscopic sources situations occur where it to a good approximation can be assumed that the source dynamics relates to a single particle. We shall further assume that only bound states are important for the electrodynamics. If, as usual, we denote the bound electron energy eigenfunctions by $|i\rangle, |j\rangle, \dots$, the completeness theorem takes the form

$$\sum_i |i\rangle \langle i| = \hat{1} \quad (27.21)$$

in the particle state space. With the help of (27.21) the transverse current density operator can be written in the form

$$\hat{\mathbf{J}}_T = \hat{1} \hat{\mathbf{J}}_T \hat{1} = \sum_{i,j} \langle j | \hat{\mathbf{J}}_T | i \rangle (|j\rangle \langle i|). \quad (27.22)$$

For what follows it is convenient to work in the configuration space representation, where the matrix elements of $\hat{\mathbf{J}}_T$ and $\hat{\mathbf{J}}$ are connected via

$$\langle j | \hat{\mathbf{J}}_T | i \rangle(\mathbf{r}, t) = \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \langle j | \hat{\mathbf{J}} | i \rangle(\mathbf{r}', t) d^3 r'. \quad (27.23)$$

If the wave functions of the stationary states are denoted by $u_i(\mathbf{r}) \equiv \langle \mathbf{r} | i \rangle$, $u_j(\mathbf{r}, t) \equiv \langle \mathbf{r} | j \rangle$, etc., the transition current density (operator) from state i to state j is given by

$$\begin{aligned} \hat{\mathbf{J}}_{i \rightarrow j}(\mathbf{r}, t) \equiv \langle j | \hat{\mathbf{J}} | i \rangle(\mathbf{r}, t) &= -\frac{e\hbar}{2im} (u_j^*(\mathbf{r}) \nabla u_i(\mathbf{r}) \\ &\quad - u_i(\mathbf{r}) \nabla u_j^*(\mathbf{r})) - \frac{e^2}{m} \hat{\mathbf{A}}_T(\mathbf{r}, t) u_i(\mathbf{r}) u_j^*(\mathbf{r}), \end{aligned} \quad (27.24)$$

where $-e$ and m are the electron charge and rest mass. Before proceeding a few remarks should be given to (27.24). As indicated, the transition current density is still an operator. This is so because $\hat{\mathbf{J}}$ is an operator in the state space $\mathcal{E}$ of the global field-particle system. The matrix element of $\hat{\mathbf{J}}$, $\langle j | \hat{\mathbf{J}} | i \rangle$, is taken between states in the particle state space, $\mathcal{E}_P$, and this leaves us with an operator in the state space $\mathcal{E}_F$ of the radiation field. In (27.24) this fact manifests itself by the presence of the transverse vector potential, $\hat{\mathbf{A}}_T(\mathbf{r}, t)$. Although the transition current density operator, as we know from the analysis in Sects. 11.5 and 11.6, is gauge invariant, the *explicit* expression given on the right-hand-side of (27.24) belongs to the Coulomb gauge, cf. (11.129) and (11.130). To recapitulate: A gauge transformation changes the phase of the wave function (see (11.175)) locally. For a certain phase change $(q/\hbar)\chi(\mathbf{r}, t)$, the terms containing the gradient $\nabla\chi(\mathbf{r}, t)$ in (11.130) cancel the term proportional to the longitudinal part of the vector potential. Since $\langle j | \hat{\mathbf{J}} | i \rangle$ is gauge invariant so is $\langle j | \hat{\mathbf{J}}_T | i \rangle$. The gauge invariance of $\langle j | \hat{\mathbf{J}}_T | i \rangle$ is manifest from (27.1) because $\hat{\mathbf{A}}_T$ is the same in every gauge.

The operator

$$\hat{b}_{i \rightarrow j}(t) \equiv |j\rangle \langle i|(t) \quad (27.25)$$

appearing in (27.22) is the so-called flip operator belonging to the transition $i \rightarrow j$. It is named so, because it when acting on the state $|i\rangle$ transforms it into the state $|j\rangle$. In the Heisenberg picture (used here) the $\hat{b}_{i \rightarrow j}$'s are time dependent, as already indicated in the notation of (27.25). Readers familiar with the quantization procedure for the electron wave-field (second-quantization) may have realized that the form given on the right-hand-side of (27.22) for $\hat{\mathbf{J}}_T$ relates to second quantization. In brief: The Schrödinger field $\psi(\mathbf{r}, t)$ may be quantized by replacing the time dependent

$c_i(t)$ -coefficients in the expansion

$$\psi(\mathbf{r}, t) = \sum_i c_i(t) u_i(\mathbf{r}) \quad (27.26)$$

by what becomes electron annihilation operators $\hat{c}_i(t)$. The wave function $\psi(\mathbf{r}, t)$ in consequence also becomes an operator

$$\hat{\psi}(\mathbf{r}, t) = \sum_i \hat{c}_i(\mathbf{r}, t) u_i(\mathbf{r}). \quad (27.27)$$

In the second-quantized (SQ) formalism the transverse current density operator is given by

$$\hat{\mathbf{J}}_T(\mathbf{r}, t; \text{SQ}) = \int_{-\infty}^{\infty} \hat{\psi}^\dagger(\mathbf{r}_e, t) \hat{\mathbf{J}}_T(\mathbf{r}, \mathbf{r}_e, t; \text{FQ}) \hat{\psi}(\mathbf{r}_e, t) d^3 r_e, \quad (27.28)$$

where $\hat{\mathbf{J}}_T(\mathbf{r}, \mathbf{r}_e, t; \text{FQ})$ is the transverse current density operator in first-quantized (FQ) form. The explicit expression for this last operator follows from the single-particle form of (23.149), with the electron coordinate denoted by $\mathbf{r}_e$. A combination of (23.149), (27.27) and (27.28) gives

$$\hat{\mathbf{J}}_T(\mathbf{r}, t; \text{SQ}) = \sum_{i,j} \langle j | \hat{\mathbf{J}}_{T(\text{FQ})} | i \rangle \hat{c}_j^\dagger(t) \hat{c}_i(t), \quad (27.29)$$

and by comparison to (27.22) (with (27.25) inserted) it appears that the flip operator is just

$$\hat{b}_{i \rightarrow j}(t) = \hat{c}_j^\dagger(t) \hat{c}_i(t). \quad (27.30)$$

In the language of second quantization, the flip operator relates to a double process where we annihilate an electron in state i , and create one in state j . In connection to our study of the electrodynamics of the two-level atom in Sect. 27.4 we shall have more to say on the flip operator.

27.2.2 The Retarded Relation Between Field and Flip Operators

In view of the considerations on the transverse current density operator, we can now conclude that the integral relation in (27.1) can be rewritten as follows:

$$\hat{\mathbf{A}}_T(\mathbf{r}, t) = \hat{\mathbf{A}}_T^{\text{ext}}(\mathbf{r}, t) + \mu_0 \sum_{i,j} \int_{-\infty}^{\infty} g(R, \tau) \langle j | \hat{\mathbf{J}}_T | i \rangle (\mathbf{r}', t') \hat{b}_{i \rightarrow j}(t') dt' d^3 r', \quad (27.31)$$

or equivalently as

$$\hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t) = \hat{\mathbf{A}}_{\text{T}}^{\text{ext}}(\mathbf{r}, t) + \frac{\mu_0}{4\pi} \sum_{i,j} \int_{-\infty}^{\infty} \frac{1}{|\mathbf{r} - \mathbf{r}'|} \langle j | \hat{\mathbf{J}}_{\text{T}} | i \rangle (\mathbf{r}', t_{\text{ret}}) \hat{b}_{i \rightarrow j}(t_{\text{ret}}) d^3 r', \quad (27.32)$$

where

$$t_{\text{ret}} = t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0} \quad (27.33)$$

is the retarded time related to $\mathbf{r}$ and $\mathbf{r}'$. The result in (27.32) relates, in the Heisenberg picture, the transverse vector potential operator of the quantized electromagnetic field to the various atomic flip operators. It must be remembered that $\hat{\mathbf{A}}_{\text{T}}$ not only appears on the left side of the equation, but also in the matrix element $\langle j | \hat{\mathbf{J}}_{\text{T}} | i \rangle$; cf. (27.23) and (27.24).

27.2.3 Single-Electron Spontaneous Emission: Neglect of Diamagnetism

A theory of spontaneous emission cannot be established without taking into account the fact that the speed of light is finite. What is needed for the calculation is the field retardation across the transverse current density domain of the source. However, if the source is of mesoscopic size or smaller, it is in general sufficient to treat the field retardation to lowest order. Such an approximation led to an integral relation between the retarded part of the transverse vector potential and the source current density of the form given in (27.5). For a single-electron source the current density operator is given by

$$\hat{\mathbf{J}}(\mathbf{r}, t) = \sum_{i,j} \langle j | \hat{\mathbf{J}} | i \rangle (\mathbf{r}, t) \hat{b}_{i \rightarrow j}(t). \quad (27.34)$$

In the lowest-order calculation only the integral of the transition current density operator $\langle j | \hat{\mathbf{J}} | i \rangle$ (27.24) over the source domain is needed. If the variation of the total transverse vector potential across the source domain is neglected the diamagnetic part of the transition current density does not contribute to the spontaneous emission process. Thus, with the source located around $\mathbf{r} = \mathbf{0}$, one obtains

$$\int_{-\infty}^{\infty} \hat{\mathbf{A}}_{\text{T}}(\mathbf{r}, t) u_i(\mathbf{r}) u_j^*(\mathbf{r}) d^3 r \approx \hat{\mathbf{A}}_{\text{T}}(\mathbf{0}, t) \int_{-\infty}^{\infty} u_i(\mathbf{r}) u_j^*(\mathbf{r}) d^3 r = \mathbf{0}, \quad (27.35)$$

since the energy eigenstates are mutually orthogonal. In view of (27.35) one has approximately

$$\hat{\mathbf{J}}(\mathbf{r}, t) = \sum_{i,j} \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) \hat{b}_{i \rightarrow j}(t), \quad (27.36)$$

where

$$\mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) = -\frac{e\hbar}{2im} (u_j^*(\mathbf{r}) \nabla u_i(\mathbf{r}) - u_i(\mathbf{r}) \nabla u_j^*(\mathbf{r})) \quad (27.37)$$

is the gauge invariant paramagnetic transition current density from state i to state j (given before in (12.61)). With the abbreviation

$$\mathbf{J}_{i \rightarrow j}^{\text{ED}} \equiv \int_{-\infty}^{\infty} \mathbf{j}_{i \rightarrow j}^0(\mathbf{r}) d^3 r, \quad (27.38)$$

the important integral relation in (27.9) finally becomes

$$\hat{\mathbf{A}}_{\text{T}}^{\text{spon}}(\mathbf{0}, t) = -\frac{\mu_0}{6\pi c_0} \sum_{i,j} \mathbf{J}_{i \rightarrow j}^{\text{ED}} \frac{d}{dt} \hat{b}_{i \rightarrow j}(t). \quad (27.39)$$

In the terminology used in Sect. 5.1, the quantity $\mathbf{J}_{i \rightarrow j}^{\text{ED}}$ may be characterized as the electric-dipole current density associated with the transition $i \rightarrow j$, cf. (5.7). As in the classical case (5.6), $\mathbf{J}_{i \rightarrow j}^{\text{ED}}$ has the dimension of a current density times a volume. The $\mathbf{J}_{i \rightarrow j}^{\text{ED}}$ -vector is closely related to the matrix element of the electric-dipole operator $-e\hat{\mathbf{r}}$ ($= -e\mathbf{r}$ in the configuration space representation) between the states i and j . In order to find this connection, one makes use of the commutator relation

$$[\hat{\mathbf{r}}, \hat{H}_{\text{p}}^{\text{C}}] = -\frac{\hbar^2}{m} \nabla, \quad (27.40)$$

where $\hat{H}_{\text{p}}^{\text{C}}$ is the particle Hamilton operator in the Coulomb gauge (25.79). I urge the reader to prove the correctness of (27.40) to himself. By insertion of (27.37) into (27.38), one obtains upon a partial integration of the last term

$$\mathbf{J}_{i \rightarrow j}^{\text{ED}} = -\frac{e\hbar}{im} \int_{-\infty}^{\infty} u_j^*(\mathbf{r}) \nabla u_i(\mathbf{r}) d^3 r, \quad (27.41)$$

and then by means of (27.40)

$$\mathbf{J}_{i \rightarrow j}^{\text{ED}} = \frac{e}{i\hbar} \int_{-\infty}^{\infty} u_j^*(\mathbf{r}) [\hat{\mathbf{r}}, \hat{H}_{\text{p}}^{\text{C}}] u_i(\mathbf{r}) d^3 r. \quad (27.42)$$

Since the energy eigenstates ($\alpha = i, j, \dots$) satisfy the eigenvalue equation

$$\hat{H}_{\text{p}}^{\text{C}} u_{\alpha}(\mathbf{r}) = \epsilon_{\alpha} u_{\alpha}(\mathbf{r}), \quad (27.43)$$

ϵ_{α} being the energy of state α , one finally gets

$$\mathbf{J}_{i \rightarrow j}^{\text{ED}} = \frac{\epsilon_j - \epsilon_i}{i\hbar} \mathbf{d}_{i \rightarrow j}, \quad (27.44)$$

where

$$\mathbf{d}_{i \rightarrow j} \equiv \int_{-\infty}^{\infty} u_j^*(\mathbf{r}) (-e\mathbf{r}) u_i(\mathbf{r}) d^3 r \quad (27.45)$$

is the matrix element of the electric dipole operator (for a single electron) between the initial state i and the final state j . It should be noticed that the relation in (27.44) would be the same in the Poincaré gauge, because the commutator of $\hat{\mathbf{r}}$ and $\hat{H}_P^P$ also equals $(-\hbar^2/m)\nabla$. This is so since the last (c -number) term in (25.75) commutes with $\hat{\mathbf{r}}$. The connection of the Coulomb and Poincaré gauge descriptions to the electrodynamics in the so-called electric dipole approximation, where $\mathbf{d}_{i \rightarrow j}$ appears in a manifest manner, is analyzed in the following section.

27.3 The Electric Dipole Hamiltonian and the Associated Operator

27.3.1 Long-Wavelength Approximation of the Classical Poincaré Hamiltonian

In a somewhat sketchy manner we now derive the electric dipole Hamiltonian starting from the Poincaré gauge. One cannot overemphasize the importance of the electric dipole approximation for studies of electrodynamics of highly localized systems. By highly localized we mean that the spatial extension of the system should be so small that one in a first approximation can neglect that spatial variation of the various fields across the particle domain. For the vector potential we thus in the Poincaré gauge put

$$\mathbf{A}^P(\mathbf{r}_\alpha) \approx \mathbf{A}^P(\mathbf{0}) = \mathbf{0}. \quad (27.46)$$

The last member of (27.46) follows immediately from (25.17). In the interaction Hamiltonian given in (25.77) the last two sums therefore vanish. The first member of (27.46) shows that the magnetic field $\mathbf{B}(\mathbf{r}_\alpha) = \nabla_\alpha \times \mathbf{A}^P(\mathbf{r}_\alpha)$ vanishes in the particle domain. With $\mathbf{D}(\mathbf{r}_\alpha) \approx \mathbf{D}(\mathbf{0})$, and in view of (25.82), the interaction Hamiltonian thus is reduced to

$$H_I^{\text{ED}} = -\frac{1}{\epsilon_0} \mathbf{D}(\mathbf{0}) \cdot \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}) d^3r. \quad (27.47)$$

By means of (25.20) it appears that the volume integral $\mathbf{P}(\mathbf{r})$, viz.,

$$\mathbf{d} \equiv \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}) d^3r = \sum_{\alpha} q_{\alpha} \mathbf{r}_{\alpha}, \quad (27.48)$$

is just the electric dipole moment of the charge distribution. In the long-wavelength limit the interaction Hamiltonian hence takes the form

$$H_I^{\text{ED}} = -\frac{1}{\epsilon_0} \mathbf{d} \cdot \mathbf{D}(\mathbf{0}). \quad (27.49)$$

If one neglects the field generated by the particle system itself, and thus assumes that $\mathbf{D}(\mathbf{0})$ is the $\mathbf{D}$ -field originating in external sources located outside the system,

one obtains

$$H_I^{\text{ED}} \approx -\mathbf{d} \cdot \mathbf{E}^{\text{ext}}(\mathbf{0}), \quad (27.50)$$

i.e., the familiar textbook interaction Hamiltonian.

Let us now consider the particle Hamiltonian H_p^p , given in (25.75). Since the magnetic field acting on the particle system vanishes in the long-wavelength limit, the canonical momentum of the individual particles, $\mathbf{p}_\alpha^p$, equals $m_\alpha \dot{\mathbf{r}}_\alpha$ (see (25.65)), and the first term on the right side of (25.75) therefore truly represents the kinetic energy of the particles. Since, the polarization in the ED-approximation, $\mathbf{P}^{\text{ED}}(\mathbf{r})$, is given by

$$\mathbf{P}^{\text{ED}}(\mathbf{r}) = \delta(\mathbf{r}) \int_{-\infty}^{\infty} \mathbf{P}(\mathbf{r}) d^3r = \mathbf{d} \delta(\mathbf{r}), \quad (27.51)$$

the transverse polarization entering (25.75) must be approximated by

$$\mathbf{P}_T^{\text{ED}}(\mathbf{r}) = \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \mathbf{d} \delta(\mathbf{r}') d^3r' = \delta_T(\mathbf{r}) \cdot \mathbf{d}. \quad (27.52)$$

In the ED-limit the last term of (25.75) hence is given by

$$\frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_T^2(\mathbf{r}) d^3r = \frac{1}{2\epsilon_0} \mathbf{d} \cdot \left[\int_{-\infty}^{\infty} \delta_T(\mathbf{r}) \cdot \delta_T(\mathbf{r}) d^3r \right] \cdot \mathbf{d}. \quad (27.53)$$

The reader may readily realize that the integral of the product of the transverse delta functions equals $\delta_T(\mathbf{0})$. The term

$$\frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_T^2(\mathbf{r}) d^3r = \frac{1}{2\epsilon_0} \mathbf{d} \cdot \delta_T(\mathbf{0}) \cdot \mathbf{d} \quad (27.54)$$

in the particle Hamiltonian therefore seems to diverge. To examine this problem closer, let us now consider the (divergent) mode expansion of $\delta_T(\mathbf{0})$, namely

$$\delta_T(\mathbf{0}) = \int_{-\infty}^{\infty} (U - \kappa\kappa) \frac{d^3q}{(2\pi)^3} \Rightarrow L^{-3} \sum_q (U - \kappa\kappa) = L^{-3} \sum_{q,s} \epsilon_{qs} \epsilon_{qs}. \quad (27.55)$$

It is apparent from (27.55) that the divergence stems from the inclusion of infinitely many $\mathbf{q}$ -modes. In fact, one must limit the sum to $\mathbf{q}$ -values for which the long-wavelength approximation is valid. By including only modes with $|\mathbf{q}| < q_M$, one obtains in the discrete mode expansion the non-divergent result

$$\frac{1}{2\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_T^2(\mathbf{r}) d^3r \approx \frac{1}{2\epsilon_0 L^3} \sum_{q,s} (\epsilon_{qs} \cdot \mathbf{d})^2, \quad q < q_M. \quad (27.56)$$

Since the transverse delta function equals $(2/3)U\delta(\mathbf{0})$ at the origo, (27.54) may also be given in the form

$$\frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}_T^2(\mathbf{r}) d^3r = \frac{1}{3\epsilon_0} \mathbf{d} \cdot \mathbf{d} \delta(\mathbf{0}). \quad (27.57)$$

Physically, the reader may recognize the expression on the right side of this equation as the (infinite) self-energy of the electric dipoles of the system. The Coulomb energy, V_{Coul} , is unaffected by the long-wavelength approximation, but it must be remembered that the Coulomb self-energy of the individual particles is infinite, unless one introduces a cutoff in the integral over $\mathbf{q}$ -space, cf. the analysis in Sect. 9.3.2.

The field Hamiltonian, H_F^P , given in (25.76) involves a knowledge of the field quantities $\mathbf{D}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ over the entire space, and for this reason H_F^P stays unaltered in the transition to the ED-approximation. Altogether, our nonrigorous considerations have led to the following classical ED-Hamiltonian:

$$\begin{aligned} H^{\text{ED}} = & \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{\mathbf{r}}_{\alpha}^2 + V_{\text{Coul}} + \frac{1}{2\epsilon_0 L^3} \sum_{q,s} (\epsilon_{qs} \cdot \mathbf{d})^2 \\ & + \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[\left(\frac{\mathbf{D}(\mathbf{r})}{\epsilon_0} \right)^2 + c_0^2 \mathbf{B}^2(\mathbf{r}) \right] d^3r - \frac{1}{\epsilon_0} \mathbf{d} \cdot \mathbf{D}(\mathbf{0}), \quad q < q_M. \end{aligned} \quad (27.58)$$

The correctness of the result above is justified in the following.

27.3.2 Long-Wavelength Unitary Transformation of the Coulomb Hamilton Operator

We now turn the attention towards the quantum electrodynamic description in the long-wavelength limit. The analysis starts from the Coulomb Hamiltonian in the Schrödinger representation, where all operators are time independent. If, as in the classical description, we neglect the variation of the field operators across the source domain, the vector-potential operator in (23.47) is replaced by

$$\hat{\mathbf{A}}_T(\mathbf{0}) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} (\hat{a}_{qs} + \hat{a}_{qs}^{\dagger}) \epsilon_{qs}, \quad (27.59)$$

and the Coulomb Hamiltonian in (23.83) by

$$\begin{aligned} \hat{H} = & \sum_{\alpha} \frac{1}{2m_{\alpha}} \left(\hat{\mathbf{p}}_{\alpha} - q_{\alpha} \hat{\mathbf{A}}_T(\mathbf{0}) \right)^2 + \hat{V}_{\text{Coul}} \\ & + \sum_{q,s} \hbar \omega_q \left(\hat{a}_{qs}^{\dagger} \hat{a}_{qs} + \frac{1}{2} \right). \end{aligned} \quad (27.60)$$

In the previous subsection, we reached the classical electric-dipole Hamiltonian by a long-wavelength approximation in the Poincaré gauge, and in Sect. 25.5.2 a unitary transformation ((25.95) with (25.96) inserted) transferred the quantum description from the Coulomb to the Poincaré gauge. Inspired by the two aforementioned aspects, we apply the unitary transformation one obtains by replacing $\hat{A}_T(\mathbf{r})$ in (25.96) by $\hat{A}_T(\mathbf{0})$, i.e.,

$$\begin{aligned}\hat{T} &= \exp \left[-\frac{i}{\hbar} \left(\int_{-\infty}^{\infty} \hat{\mathbf{P}}(\mathbf{r}) d^3r \right) \cdot \hat{\mathbf{A}}_T(\mathbf{0}) \right] \\ &= \exp \left(-\frac{i}{\hbar} \hat{\mathbf{d}} \cdot \hat{\mathbf{A}}_T(\mathbf{0}) \right),\end{aligned}\quad (27.61)$$

to the Coulomb Hamiltonian. The operator $\hat{\mathbf{d}}$ is the electric dipole operator of the particles, and in the $\{\mathbf{r}\}$ -representation, where $\hat{\mathbf{r}}_\alpha = \mathbf{r}_\alpha$, it is given by (27.48). Before subjecting $\hat{H}$ to the transformation in (27.61), it is stressed that since $\hat{\mathbf{A}}_T(\mathbf{0})$ and $\hat{\mathbf{d}}$ in the Schrödinger picture are time independent, so will $\hat{T}$ be. From (25.90) it then follows that the Hamiltonians in the new (2) and old (1) descriptions are related by

$$\hat{H}^{(2)} = \hat{T} \hat{H}^{(1)} \hat{T}^\dagger, \quad (27.62)$$

and that $\hat{H}^{(2)}$ is independent of time.

Consider first the transformation of the various particle and field operators entering (27.60). Since,

$$\hat{T} \hat{\mathbf{A}}_T(\mathbf{0}) \hat{T}^\dagger = \hat{\mathbf{A}}_T(\mathbf{0}), \quad (27.63)$$

obviously, and

$$\hat{T} \hat{\mathbf{p}}_\alpha \hat{T}^\dagger = \hat{\mathbf{p}}_\alpha + q_\alpha \hat{\mathbf{A}}_T(\mathbf{0}), \quad (27.64)$$

one gets

$$\begin{aligned}\hat{T} \left(\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\mathbf{0}) \right)^2 \hat{T}^\dagger \\ &= \hat{T} \left(\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\mathbf{0}) \right) \hat{T}^\dagger \cdot \hat{T} \left(\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\mathbf{0}) \right) \hat{T}^\dagger \\ &= \hat{\mathbf{p}}_\alpha^2.\end{aligned}\quad (27.65)$$

In the new representation, where

$$\hat{T} \left[\sum_\alpha \frac{1}{2m_\alpha} \left(\hat{\mathbf{p}}_\alpha - q_\alpha \hat{\mathbf{A}}_T(\mathbf{0}) \right)^2 \right] \hat{T}^\dagger = \sum_\alpha \frac{1}{2m_\alpha} \hat{\mathbf{p}}_\alpha^2, \quad (27.66)$$

$\hat{\mathbf{p}}_\alpha/m_\alpha$ is just the velocity operator of particle α . Because the potential energy $\hat{V}_{\text{Coul}}$ is not changed by the transformation, the operator

$$\hat{H}_p^{\text{Proper}} = \sum_\alpha \frac{1}{2m} \hat{\mathbf{p}}_\alpha^2 + \hat{V}_{\text{Coul}} \quad (27.67)$$

represents the proper energy of the particles in the new description. Since

$$\hat{T} \hat{a}_{qs}^\dagger \hat{a}_{qs} \hat{T}^\dagger = \hat{T} \hat{a}_{qs}^\dagger \hat{T}^\dagger \hat{T} \hat{a}_{qs} \hat{T}^\dagger, \quad (27.68)$$

the radiation part of the Coulomb Hamiltonian is easily transformed when the transforms of $\hat{a}_{qs}$ and $\hat{a}_{qs}^\dagger$ have been obtained. To transform these, we first insert the expansion for $\hat{A}_T(\mathbf{0})$ (27.59) into (27.61). This gives

$$\hat{T} = \exp \left[\sum_{q,s} \left(\hat{\eta}_{qs}^\dagger \hat{a}_{qs} - \hat{\eta}_{qs} \hat{a}_{qs}^\dagger \right) \right], \quad (27.69)$$

where

$$\hat{\eta}_{qs} \equiv i \left(2\epsilon_0 \hbar \omega_q L^3 \right)^{-1/2} \hat{\mathbf{d}} \cdot \boldsymbol{\epsilon}_{qs} \quad (27.70)$$

is a pure particle operator. Since the operator acts like a c -number with respect to the field operators, we just write $\hat{\eta}_{qs} = \eta_{qs}$ and $\hat{\eta}_{qs}^\dagger = \eta_{qs}^*$ [in the $\{\mathbf{r}\}$ -representation] in what follows. By utilizing (23.41) and (23.42) one obtains

$$\hat{T} \hat{a}_{qs} \hat{T}^\dagger = \exp \left(\eta_{qs}^* \hat{a}_{qs} - \eta_{qs} \hat{a}_{qs}^\dagger \right) \hat{a}_{qs} \exp \left(\eta_{qs} \hat{a}_{qs}^\dagger - \eta_{qs}^* \hat{a}_{qs} \right). \quad (27.71)$$

Since the commutator

$$\left[\eta_{qs}^* \hat{a}_{qs} - \eta_{qs} \hat{a}_{qs}^\dagger, \hat{a}_{qs} \right] = \eta_{qs} \quad (27.72)$$

is a c -number in the field subspace, the operator expansion theorem (25.115) immediately gives

$$\hat{T} \hat{a}_{qs} \hat{T}^\dagger = \hat{a}_{qs} + \eta_{qs}, \quad (27.73)$$

and the Hermitian conjugate of this relation is

$$\hat{T} \hat{a}_{qs} \hat{T}^\dagger = \hat{a}_{qs}^\dagger + \eta_{qs}^*. \quad (27.74)$$

By a combination of (27.60) (last sum), (27.68), (27.73) and (27.74), it appears that the radiation Hamiltonian is transformed to

$$\begin{aligned} & \hat{T} \left[\sum_{q,s} \hbar \omega_q \left(\hat{a}_{qs} \hat{a}_{qs} + \frac{1}{2} \right) \right] \hat{T}^\dagger \\ &= \sum_{q,s} \hbar \omega_q \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \frac{1}{2} \right) + \sum_{q,s} \hbar \omega_q \left(\eta_{qs} \hat{a}_{qs}^\dagger + \eta_{qs}^* \hat{a}_{qs} \right) \\ &+ \sum_{q,s} \hbar \omega_q \eta_{qs}^* \eta_{qs}. \end{aligned} \quad (27.75)$$

In the new description the first sum is the radiation Hamiltonian, and the last two sums represent, as we shall soon see, the interaction Hamiltonian and the Hamiltonian related to the dipole self-energy in the long-wavelength limit, respectively. Since

$$\sum_{q,s} \hbar \omega_q \left(\eta_{qs} \hat{a}_{qs}^\dagger + \eta_{qs}^* \hat{a}_{qs} \right) = \mathbf{d} \cdot \left[\sum_{q,s} i \left(\frac{\hbar \omega}{2\epsilon_0 L^3} \right)^{1/2} \left(\hat{a}_{qs}^\dagger - \hat{a}_{qs} \right) \boldsymbol{\epsilon}_{qs} \right], \quad (27.76)$$

and the term in the sharp parenthesis multiplied by minus one is just the long-wavelength limit of the transverse electric field operator in the old (Coulomb) representation; cf. (23.49), (25.120) tells us that

$$\sum_{q,s} \hbar \omega_q \left(\eta_{qs} \hat{a}_{qs}^\dagger + \eta_{qs}^* \hat{a}_{qs} \right) = -\frac{1}{\epsilon_0} \hat{\mathbf{d}} \cdot \hat{\mathbf{D}}(\mathbf{0}) \quad (27.77)$$

where, with omission of the superscript NEW, $\hat{\mathbf{D}}(\mathbf{0})$ is the $\hat{\mathbf{D}}$ -field operator in the long-wavelength limit. The contribution in (27.77) hence represents the interaction Hamiltonian in the new description, and in the view of (27.49), it is seen to be an electric-dipole Hamiltonian coupling the dipole moment of the particles [$\hat{\mathbf{d}} = \hat{\mathbf{d}}^{\text{NEW}}$] to the electric displacement field at the origo. The last sum in (27.75) gives with the help of (27.70)

$$\sum_{q,s} \hbar \omega_q \eta_{qs}^* \eta_{qs} = \frac{1}{2\epsilon_0 L^3} \sum_{q,s} \left(\boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{d}} \right)^2, \quad (27.78)$$

and this is precisely the operator belonging to the self-energy of the electric dipoles of the system. In conclusion, the new (electric-dipole) Hamilton operator is found to have the form

$$\begin{aligned} \hat{H}^{\text{ED}} = & \sum_{\alpha} \frac{\hat{\mathbf{p}}_{\alpha}^2}{2m_{\alpha}} + \hat{V}_{\text{Coul}} + \frac{1}{2\epsilon_0 L^3} \sum_{q,s} \left(\boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{d}} \right)^2 \\ & + \sum_{q,s} \hbar \omega_q \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \frac{1}{2} \right) - \frac{1}{\epsilon_0} \hat{\mathbf{d}} \cdot \hat{\mathbf{D}}(\mathbf{0}), \end{aligned} \quad (27.79)$$

(with $q < q_M$ in the dipole's self-energy term), in complete agreement with what one could expect on the basis of the classical Hamiltonian in (27.58).

27.4 Two-Level Atom

The description of the interaction between a quantized electromagnetic field and a single atom is one of the most fundamental objectives of quantum optics, and theoretical methods developed in this subfield of physical optics have, and can, often be

employed in studies of quantum electrodynamic phenomena in more complicated systems, such as molecules and mesoscopic particles. However, atoms are complicated quantum objects, and even the most simple atom, hydrogen, has a non-trivial energy level structure. For many purposes only two energy levels play a significant role in the electrodynamic interaction. This may be the case, for instance, when (quasi-) monochromatic light interacts resonantly with a given atomic transition, and the other levels are far away, or the interaction with the neighboring levels is forbidden by the selection rules. It is perhaps surprising that the two-level approximation sometimes is fruitful even in solid-state electrodynamics. In what follows, we shall use the name “two-level atom” for all mesoscopic and microscopic systems, which in a given situation, behave like two-level quantum objects, and we shall assume that the electrodynamic interaction can be described accurately in the electric-dipole approximation.

27.4.1 Raising and Lowering Operators

Let us thus consider a two-level atom for which the energy levels are separated by an amount $\hbar\omega_0$, and let us choose the energy axis in such a manner that the energy is zero midway between the two levels. The lower ($|1\rangle$) and higher ($|2\rangle$) energy eigenstates therefore have the energies $E_1 = -\hbar\omega_0/2$ and $E_2 = \hbar\omega_0/2$, respectively, and if we denote the particle part of the electric-dipole Hamiltonian in (27.79) for a single electron bound to a fixed nucleus by $\hat{H}_p^{\text{ED}}$, the eigenvalue equations read

$$\hat{H}_p^{\text{ED}}|i\rangle = E_i|i\rangle, \quad i = 1, 2. \quad (27.80)$$

In the two-level approximation the eigenstates satisfy the orthonormality condition

$$\langle i|j\rangle = \delta_{ij}, \quad i, j = 1, 2, \quad (27.81)$$

and the completeness theorem

$$\sum_{i=1}^2 |i\rangle\langle i| = \hat{1}. \quad (27.82)$$

The flip operators, defined in (27.25), are given and abbreviated for the present case as follows:

$$\hat{b}_{1\rightarrow 2} = |2\rangle\langle 1| \equiv \hat{b}^\dagger, \quad (27.83)$$

$$\hat{b}_{2\rightarrow 1} = |1\rangle\langle 2| \equiv \hat{b}. \quad (27.84)$$

The operators $\hat{b}$ and $\hat{b}^\dagger$ lower and raise the atomic excitation, i.e.,

$$\hat{b}|2\rangle = |1\rangle, \quad \hat{b}^\dagger|1\rangle = |2\rangle, \quad (27.85)$$

and are therefore also called lowering and raising operators. Besides the relations in (27.85) they satisfy

$$\hat{b}|1\rangle = \hat{b}^\dagger|2\rangle = 0. \quad (27.86)$$

The results in (27.85) and (27.86) follow directly from the orthonormality condition (27.81). This condition also implies that the lowering and raising operators satisfy the anticommutator rules

$$\{\hat{b}, \hat{b}\} = \{\hat{b}^\dagger, \hat{b}^\dagger\} = 0, \quad (27.87)$$

$$\{\hat{b}, \hat{b}^\dagger\} = \hat{1}, \quad (27.88)$$

as the reader may verify. The relations in (27.87) and (27.88) are characteristic of Fermion algebra, see also Sect. 27.4.3.

27.4.2 Pauli Operators

A quantum system with only two energy levels is in a sense mathematically equivalent to a spin-1/2 system in a magnetic field. It is, therefore, not surprising that the Pauli spin operators are useful in studies of the dynamics of two-level atoms. In the atomic case we will use the name “Pauli operators” for these operators. In terms of $\hat{b}$ and $\hat{b}^\dagger$, the three Hermitian Pauli operators are given by

$$\hat{\sigma}_1 = \hat{b} + \hat{b}^\dagger, \quad (27.89)$$

$$\hat{\sigma}_2 = i(\hat{b} - \hat{b}^\dagger), \quad (27.90)$$

$$\hat{\sigma}_3 = \hat{b}^\dagger \hat{b} - \hat{b} \hat{b}^\dagger. \quad (27.91)$$

The three Pauli operators together with the identity operator

$$\hat{\sigma}_0 \equiv \hat{1} = \hat{b} \hat{b}^\dagger + \hat{b}^\dagger \hat{b} \quad (27.92)$$

form a complete set of linearly independent Hermitian operators in the two-dimensional Hilbert space of the atom, as the reader may verify. In consequence any two-level atomic observable, $\hat{O}$, can therefore be expanded in terms of this set, i.e.,

$$\hat{O} = \sum_{i=0}^3 \alpha_i \hat{\sigma}_i, \quad (27.93)$$

where the α_i -coefficients are determined by $\hat{O}$. In the $\{|1\rangle, |2\rangle\}$ -basis, where the matrix elements of the lowering and raising operators are related by

$$\langle i | \hat{b} | j \rangle = \left(\langle j | \hat{b}^\dagger | i \rangle \right)^*, \quad (27.94)$$

Equations (27.83) and (27.84) immediately give us the following matrix representation for $\hat{b}$ and $\hat{b}^\dagger$:

$$\hat{b} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \hat{b}^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (27.95)$$

When these matrix forms are inserted into (27.89)–(27.91) one obtains precisely the matrix representations of the Pauli spin operators; see the equations in (11.112).

27.4.3 Electron-Field Operators

In the second-quantized description of the relativistic Dirac equation, the wave function is replaced by an electron-positron field operator, where annihilation operators appear for electrons and positrons in the various states. In the Hermitian conjugate field operator the related creation operators for the electrons and positrons are involved. In the nonrelativistic regime positrons play no role, and only creation and annihilation operators for electrons are used in the second-quantized formalism, cf. the discussion in Sect. 27.2.1. In particular for the many-body theory of solids, the nonrelativistic scheme of second quantization is useful, and there, and anywhere else is nonrelativistic physics, electron annihilation and creation operators only appear in pairs. This is so because electrons cannot be created nor destroyed in the nonrelativistic domain.

Let us consider the two-level atom, and let us denote the electron vacuum state, $|0\rangle$, as follows:

$$|0\rangle \equiv |0, 0\rangle, \quad (27.96)$$

where the first and second number on the right side refer to the lower and upper states, respectively. By acting on the vacuum state with the electron creation operators for the lower ($\hat{c}_1^\dagger$) and upper ($\hat{c}_2^\dagger$) states one obtains

$$\hat{c}_1^\dagger |0\rangle = |1, 0\rangle, \quad (27.97)$$

$$\hat{c}_2^\dagger |0\rangle = |0, 1\rangle. \quad (27.98)$$

Since the electrons are Fermions, we impose the anticommutation relations

$$\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0, \quad i, j = 1, 2, \quad (27.99)$$

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}, \quad i, j = 1, 2, \quad (27.100)$$

on the annihilation and creation operators of the two states. The Pauli exclusion principle, which states that one cannot have more than one electron in the same quantum state, is ensured by the last member of (27.99). Since the vacuum state is defined by

$$\hat{c}_i |0\rangle = 0, \quad i = 1, 2, \quad (27.101)$$

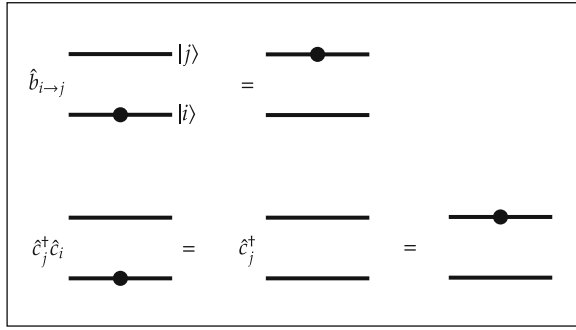


Fig. 27.1 Flip and electron-field operators. The flip operator $\hat{b}_{i \rightarrow j}$ excites an electron from the bound state $|i\rangle$ to the bound state $|j\rangle$. The same process results from the use of a combination of two electron-field operators: (1) The operator $\hat{c}_i$ annihilates the electron in state $|i\rangle$. (2) The operator $\hat{c}_j^\dagger$ creates from the vacuum (two empty states, here) an electron in state $|j\rangle$

it is not difficult to show that the quantity

$$\hat{N}_i \equiv \hat{c}_i^\dagger \hat{c}_i \quad (27.102)$$

is the number operator for state i .

The lowering and raising operators are given in terms of the electron-field operators as follows:

$$\hat{b} = \hat{c}_1^\dagger \hat{c}_2, \quad \hat{b}^\dagger = \hat{c}_2^\dagger \hat{c}_1, \quad (27.103)$$

and by means of the Fermion anticommutation relations in (27.99) and (27.100), it may be shown that the flip operators satisfy anticommutation rules of the same form; cf. (27.87) and (27.88) (see Fig. 27.1). Let us just prove (27.88), starting with the rewriting

$$\hat{b}\hat{b}^\dagger = \hat{c}_1^\dagger \hat{c}_2 \hat{c}_2^\dagger \hat{c}_1 = \hat{c}_1^\dagger \hat{c}_2 \hat{c}_1^\dagger = \hat{N}_1(\hat{1} - \hat{N}_2) = \hat{N}_1, \quad (27.104)$$

where the last member of the equation follows from the fact that $\hat{N}_1\hat{N}_2$ gives zero when it acts on an arbitrary two-level state vector. Next, we obtain

$$\hat{b}^\dagger\hat{b} = \hat{c}_2^\dagger \hat{c}_1 \hat{c}_1^\dagger \hat{c}_2 = \hat{c}_2^\dagger \hat{c}_2 \hat{c}_1^\dagger = \hat{N}_2(\hat{1} - \hat{N}_1) = \hat{N}_2. \quad (27.105)$$

By combining the results above, one finds

$$\{\hat{b}, \hat{b}^\dagger\} = \hat{N}_1 + \hat{N}_2 = \hat{N}_1 + (\hat{1} - \hat{N}_1) = \hat{1}, \quad (27.106)$$

q.e.d.

27.4.4 Electric-Dipole Hamiltonian

We finish our preliminary considerations of the two-level atom by setting up the Hamilton operator for a two-level atom interacting with a quantized electromagnetic field containing only modes of so long wavelengths that the electric-dipole approximation can be used. Implicitly, it is required that the transition between the two states is ED-allowed.

Since

$$\langle j | \hat{H}_p^{\text{ED}} | i \rangle = E_i \delta_{ij}, \quad (27.107)$$

we obtain for the particle Hamiltonian

$$\begin{aligned} \hat{H}_p^{\text{ED}} &= \sum_{i,j=1}^2 |j\rangle \langle j | \hat{H}_p^{\text{ED}} | i \rangle \langle i| = \frac{1}{2} \hbar \omega_0 (|2\rangle \langle 2| - |1\rangle \langle 1|) \\ &= \frac{1}{2} \hbar \omega_0 (\hat{b}^\dagger \hat{b} - \hat{b} \hat{b}^\dagger). \end{aligned} \quad (27.108)$$

The form of the radiation Hamiltonian is of course independent of the atomic structure. To determine the interaction Hamiltonian for the two-level system, let us first consider the electric-dipole operator for our single electron, i.e., $\hat{\mathbf{d}} = -e\mathbf{r}$, or

$$\hat{\mathbf{d}} = \sum_{i,j=1}^2 |j\rangle \langle j | \hat{\mathbf{d}} | i \rangle \langle i|. \quad (27.109)$$

Since the single-electron particle Hamiltonian, $\hat{H}_p^{\text{ED}}$ is invariant under spatial inversion ($\mathbf{r} \Rightarrow -\mathbf{r}$), the parity operator commutes with $\hat{H}_p^{\text{ED}}$, and all eigenstates of $\hat{H}_p^{\text{ED}}$ may therefore be assumed to have a definite parity. This implies that the diagonal elements of the dipole operator vanish, that is,

$$\langle i | -e\mathbf{r} | i \rangle = 0, \quad i = 1, 2, \quad (27.110)$$

remembering that the absolute square of the involved wave function is a symmetric function of $\mathbf{r}$. From (27.109) one hence obtains

$$\hat{\mathbf{d}} = \mathbf{d}_{1 \rightarrow 2} |2\rangle \langle 1| + \mathbf{d}_{2 \rightarrow 1} |1\rangle \langle 2|, \quad (27.111)$$

where

$$\mathbf{d}_{i \rightarrow j} = \langle j | -e\mathbf{r} | i \rangle \quad (27.112)$$

is the transition matrix element of the ED-operator from state i to j . This matrix element was introduced earlier in relation to the preliminary discussion of the spontaneous emission process (Sect. 27.2.3, (27.45)). Since $\mathbf{d}_{i \rightarrow j} = \mathbf{d}_{j \rightarrow i}^*$, (27.110) may be written in terms of the raising and lowering operators as follows:

$$\hat{\mathbf{d}} = \hat{b}^\dagger \mathbf{d}_{1 \rightarrow 2} + \hat{b} \mathbf{d}_{1 \rightarrow 2}^*. \quad (27.113)$$

The interaction Hamiltonian in the ED-approximation (27.77) then is obtained by inserting (27.113) into (27.77), and via the mode expansion of $\hat{\mathbf{D}}(0)$, we finally reach the important form

$$\hat{H}_I^{\text{ED}} = \sum_{\mathbf{q},s} \hbar \left(g_{\mathbf{q}s} \hat{b}^\dagger - g_{\mathbf{q}s}^* \hat{b} \right) \left(\hat{a}_{\mathbf{q}s} - \hat{a}_{\mathbf{q}s}^\dagger \right), \quad (27.114)$$

where

$$g_{\mathbf{q}s} = \frac{1}{i\hbar} \left(\frac{\hbar\omega_{\mathbf{q}}}{2\epsilon_0 L^3} \right)^{1/2} \mathbf{d}_{1 \rightarrow 2} \cdot \boldsymbol{\epsilon}_{\mathbf{q}s} \quad (27.115)$$

is the so-called coupling constant. As it stands, $g_{\mathbf{q}s}$ is in general a complex quantity, but since, as we shall realize now, the scalar product contains an arbitrary phase factor, it is possible to make $g_{\mathbf{q}s}$ real. Our choice of real unit vectors in the field expansion implies that the only adjustable phase factor in case must be contained in $\mathbf{d}_{1 \rightarrow 2}$, given in the configuration space representation by (27.45) [$i = 1, j = 2$]. The transition matrix element does contain such a factor since each of the stationary state wave functions only are given up to a global phase factor. Let us assume this factor is $\exp(i\Phi)$. To make the coupling constant real one must choose Φ so that $i^{-1} \exp(i\Phi)$ becomes real, cf. (27.115). This goal is achieved for $\Phi = \pi/2$. With real $g_{\mathbf{q}s}$'s, the interaction Hamiltonian becomes [$g_{\mathbf{q}s} > 0$]

$$\hat{H}_I^{\text{ED}} = \sum_{\mathbf{q},s} \hbar g_{\mathbf{q}s} \left(\hat{b}^\dagger - \hat{b} \right) \left(\hat{a}_{\mathbf{q}s} - \hat{a}_{\mathbf{q}s}^\dagger \right). \quad (27.116)$$

The interaction between the two-level atom and a given field mode ($\mathbf{q}s$), thus contains four types of processes, described via $\hat{b}^\dagger \hat{a}_{\mathbf{q}s}$, $\hat{b} \hat{a}_{\mathbf{q}s}^\dagger$, $\hat{b} \hat{a}_{\mathbf{q}s}$, and $\hat{b}^\dagger \hat{a}_{\mathbf{q}s}^\dagger$. These are illustrated schematically in Fig. 27.2. In the $\hat{b}^\dagger \hat{a}_{\mathbf{q}s}$ -process a photon is absorbed and the atom excited, and in the $\hat{b} \hat{a}_{\mathbf{q}s}^\dagger$ -process the atom is deexcited while emitting a photon. Roughly speaking, these processes are compatible with the principle of energy conservation. The two remaining processes violate energy conservation. Thus, the $\hat{b} \hat{a}_{\mathbf{q}s}$ -process corresponds to a situation where a photon is absorbed and the atom deexcited (loss of energy). In the $\hat{b}^\dagger \hat{a}_{\mathbf{q}s}^\dagger$ -process the atom is excited and a photon emitted (gain of energy). In quantum electrodynamics also the last two processes occur, because it is possible to violate the law of energy conservation in short periods of time. In studies of the interaction of a two-level atom with a single field mode, it is often for frequencies near resonance ($\omega \approx \omega_0$) possible to neglect the energy violating terms in the Hamiltonian. This is roughly speaking so because their effects vanish when averaged over a time interval longer than $\approx (\omega + \omega_0)^{-1}$. In the so-called rotating-wave approximation these antiresonant terms are left out from the beginning of the analysis.

Gathering the results obtained in this subsection, it is concluded that the ED-Hamiltonian describing the interaction of a two-level atom with the long wavelength part of the electrodynamic field can be given the form

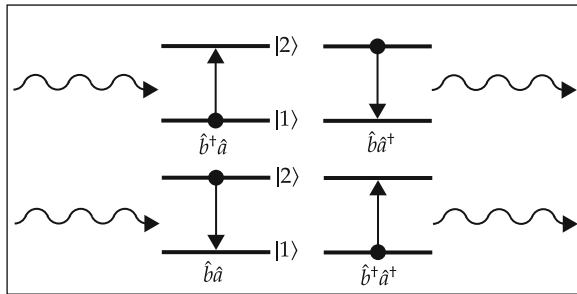


Fig. 27.2 Graphic illustration of the four fundamental quantum processes which occur in the electromagnetic interaction between a two-level atom and a single field mode. *Top left*: An incoming photon is absorbed (annihilation operator: $\hat{a}$) and the electron is excited from state $|1\rangle$ to state $|2\rangle$ (flip operator: $\hat{b}^\dagger$). *Top right*: The atom decays from $|2\rangle$ to $|1\rangle$ (flip operator: $\hat{b}$) under the emission of a photon (creation operator: $\hat{a}^\dagger$). *Bottom left*: An incoming photon is absorbed and the electron decays from $|2\rangle$ to $|1\rangle$. *Bottom right*: The electron is excited (from $|1\rangle$ to $|2\rangle$) while emitting a photon. In the rotating-wave approximation only the two energy conserving (resonant) processes (top diagrams) are kept in studies of the particle–field dynamics

$$\begin{aligned} \hat{H}^{\text{ED}} = & \frac{1}{2} \hbar \omega_0 (\hat{b}^\dagger \hat{b} - \hat{b} \hat{b}^\dagger) + \sum_{q,s} \hbar \omega_0 \left(\hat{a}_{qs}^\dagger \hat{a}_{qs} + \frac{1}{2} \right) \\ & + \sum_{qs} \hbar g_{qs} (\hat{b}^\dagger - \hat{b}) (\hat{a}_{qs} - \hat{a}_{qs}^\dagger). \end{aligned} \quad (27.117)$$

27.5 Dynamical Equations for a Coupled Two-Level Atom Plus Field System

In the previous section, we showed that the interaction between a two-level atom and a quantized electromagnetic field containing only long-wavelength modes is governed by the electric-dipole Hamiltonian in (27.117). The Hamiltonian contains the lowering and raising operators for the atom, and the annihilation and creation operators of all the field modes. In the Heisenberg picture, these operators depend on time, and the dynamical evolutions of the atom and the individual field operators are coupled via the coupling constant g_{qs} , given in (27.115), and made real by a certain choice of the global phase factor for the transition matrix element of the ED-operator.

27.5.1 Heisenberg Equation of Motion for the Atomic Flip Operator, $\hat{b}$

In order to determine the time evolution of the atomic dynamics, let us consider the Heisenberg equation of motion (23.97) for the lowering operator, $\hat{b}$, i.e.,

$$i\hbar \frac{d}{dt} \hat{b}(t) = [\hat{b}(t), \hat{H}^{\text{ED}}], \quad (27.118)$$

where $\hat{H}^{\text{ED}}$ is given by (27.117). The commutator between $\hat{b}(t)$ and the atomic part of the Hamiltonian is obtained via

$$\begin{aligned} [\hat{b}, \hat{b}^\dagger \hat{b} - \hat{b} \hat{b}^\dagger] &= [\hat{b}, 2\hat{b}^\dagger \hat{b} - 1] \\ &= 2 [\hat{b}, \hat{b}^\dagger \hat{b}] \\ &= 2 (\hat{b} - 2\hat{b}^\dagger \hat{b} \hat{b}) = 2\hat{b}. \end{aligned} \quad (27.119)$$

The first and third step in (27.119) we obtained using the anticommutator relation in (27.88), and the last step is a consequence of the fact that $\hat{b}^2 = 0$ (27.87). Hence,

$$[\hat{b}(t), \hat{H}_p^{\text{ED}}(t)] = \hbar\omega_0 \hat{b}(t). \quad (27.120)$$

The commutator of $\hat{b}(t)$ with the radiation part of the Hamiltonian is zero, and the commutator with the interaction Hamiltonian obviously gives

$$[\hat{b}(t), \hat{H}_I^{\text{ED}}(t)] = [\hat{b}(t), \hat{b}^\dagger(t)] \sum_{q,s} \hbar g_{qs} (\hat{a}_{qs}(t) - \hat{a}_{qs}^\dagger(t)). \quad (27.121)$$

By gathering the partial results obtained above, the following dynamical equation is obtained for the lowering operator:

$$\frac{d}{dt} \hat{b}(t) = -i\omega_0 \hat{b}(t) + i [\hat{b}^\dagger(t), \hat{b}(t)] \sum_{q,s} g_{qs} (\hat{a}_{qs}(t) - \hat{a}_{qs}^\dagger(t)). \quad (27.122)$$

For many applications it is useful to transform (27.122) into the integral form

$$\hat{b}(t) = \hat{b}(0)e^{-i\omega_0 t} + ie^{-i\omega_0 t} \sum_{q,s} g_{qs} \int_0^t [\hat{b}^\dagger(t'), \hat{b}(t')] (\hat{a}_{qs}(t') - \hat{a}_{qs}^\dagger(t')) e^{i\omega_0 t'} dt'. \quad (27.123)$$

It appears from this result that the time evolution of the atomic flip operator in general is very complicated.

27.5.2 Heisenberg Equation of Motion for the Field Annihilation Operator, $\hat{a}_{qs}$

The time dependence of the atomic lowering operator cannot be determined unless the time evolution of the field operators in (27.123) are known. Let us therefore now

turn our attention towards the Heisenberg equation of motion for the annihilation operator, $\hat{a}_{qs}$, viz.,

$$i\hbar \frac{d}{dt} \hat{a}_{qs}(t) = [\hat{a}_{qs}(t), \hat{H}^{\text{ED}}]. \quad (27.124)$$

We already know from (23.124) that the commutator between $\hat{a}_{qs}$ and the radiation Hamiltonian gives $\hbar\omega_q \hat{a}_{qs}$. The commutator with the atomic Hamiltonian vanishes of course. By means of the fundamental commutator relations in (23.45) and (23.46), one readily obtains for the commutator between $\hat{a}_{qs}$ and the interaction Hamiltonian

$$[\hat{a}_{qs}(t), \hat{H}_I^{\text{ED}}] = \hbar g_{qs} (\hat{b}(t) - \hat{b}^\dagger(t)). \quad (27.125)$$

Altogether, one hence obtains the following dynamical equation for the annihilation operator belonging to the (qs) -mode:

$$\frac{d}{dt} \hat{a}_{qs}(t) = -i\omega_q \hat{a}_{qs}(t) + i g_{qs} (\hat{b}^\dagger(t) - \hat{b}(t)). \quad (27.126)$$

Converted into integral form, the time dependence of $\hat{a}_{qs}$ is given by

$$\hat{a}_{qs}(t) = \hat{a}_{qs}(0)e^{-i\omega_q t} + i g_{qs} e^{-i\omega_q t} \int_0^t (\hat{b}^\dagger(t') - \hat{b}(t')) e^{i\omega_q t'} dt'. \quad (27.127)$$

Together, the coupled equations in (27.123) and (27.127) [one for each (qs) -mode] determine the time evolution of the coupled atom-field system.

27.6 Spontaneous Emission and Lamb Shift: Heuristic Approach

In the electric-dipole approximation the interaction between a two-level atom and a quantized electromagnetic field may be described in terms of a complicated set of coupled differential equations for the atomic flip operator ($\hat{b}(t)$) and the individual field annihilation operators ($\hat{a}_{qs}(t)$) ((27.122) and (27.126)). Many important physical phenomena can be studied rigorously on the basis of these equations. In the following we shall concentrate on a heuristic description of the spontaneous emission process and the Lamb shift starting from a simplified version of the coupled evolution equations.

27.6.1 Rotating-Wave Approximation

For what follows it is convenient to introduce slowly varying dynamical variables (operators) $\tilde{b}(t)$ and $\tilde{a}_{qs}(t)$ by the definitions

$$\hat{b}(t) \equiv \tilde{b}(t)e^{-i\omega_0 t}, \quad (27.128)$$

$$\hat{a}_{qs} \equiv \tilde{a}_{qs}(t)e^{-i\omega_q t}. \quad (27.129)$$

In terms of these the atomic evolution equation takes the form

$$\frac{d}{dt}\tilde{b}(t) = ie^{i\omega_0 t} \left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \sum_{q,s} g_{qs} \left(\tilde{a}_{qs}(t)e^{-i\omega_q t} - \tilde{a}_{qs}^\dagger(t)e^{i\omega_q t} \right). \quad (27.130)$$

Starting from the integral form given in (27.127), the evolution equation for the field mode operator now becomes

$$\tilde{a}_{qs}(t) = \tilde{a}_{qs}(0) + ig_{qs} \int_0^t \left[\tilde{b}^\dagger(t')e^{i(\omega_q + \omega_0)t'} - \tilde{b}(t')e^{i(\omega_q - \omega_0)t'} \right] dt', \quad (27.131)$$

with $\tilde{a}_{qs}(0) = \hat{a}_{qs}(0)$. Before proceeding, I remind the reader that the coupling constant, which was made real by a certain phase choice, is given by

$$g_{qs} = \frac{1}{\hbar} \left(\frac{\hbar\omega_q}{2\epsilon_0 L^3} \right)^{1/2} |\mathbf{d}_{1 \rightarrow 2} \cdot \boldsymbol{\epsilon}_{qs}|. \quad (27.132)$$

The integral form of the dynamical equation for $\tilde{a}_{qs}(t)$ is useful here because it by insertion into (27.130) immediately leads to an atomic evolution equation which only depends on the free-field operator $\tilde{a}_{qs}(0) \exp(-i\omega_q t)$.

Let us now omit the antiresonant terms $\sim \exp[i(\omega_q + \omega_0)t]$ from (27.130) and (27.131). This gives the following set of dynamical equations in the framework of the rotating-wave approximation

$$\frac{d}{dt}\tilde{b}(t) = i \left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \sum_{q,s} g_{qs} \tilde{a}_{qs}(t) e^{i(\omega_0 - \omega_q)t}, \quad (27.133)$$

$$\tilde{a}_{qs}(t) = \tilde{a}_{qs}(0) - ig_{qs} \int_0^t \tilde{b}(t') e^{i(\omega_q - \omega_0)t'} dt'. \quad (27.134)$$

27.6.2 Markov Approximation

By inserting (27.134) into (27.133) one obtains

$$\begin{aligned} \frac{d}{dt}\tilde{b}(t) &= ie^{i\omega_0 t} \left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \sum_{q,s} g_{qs} \tilde{a}_{qs}(0) e^{-i\omega_q t} \\ &\quad + \left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \sum_{q,s} g_{qs}^2 \int_0^t \tilde{b}(t') e^{i(\omega_q - \omega_0)(t' - t)} dt'. \end{aligned} \quad (27.135)$$

Since

$$i \sum_{q,s} g_{qs} \tilde{a}_{qs}(0) e^{-i\omega_q t} = \frac{1}{i\hbar\epsilon_0} \mathbf{d}_{1 \rightarrow 2} \cdot \hat{\mathbf{D}}_{\text{free}}^{(+)}(\mathbf{0}, t), \quad (27.136)$$

the first term on the right side of (27.135) gives the contribution to $d\tilde{b}(t)/dt$ from any *free* fields acting on the atom. Basically, the free field originates in *external* sources, but the field from an external source is not necessarily a free field. In order to qualify as a free field, the field from the external source must have been released (detached) from the source, because otherwise the time evolution would not have the form $\tilde{a}_{qs}(0) \exp(-i\omega_q t)$ for the various modes. In order to include external fields not yet released from the external source, we would have to include extra terms in the ED-Hamiltonian (27.117), viz., a source-particle Hamiltonian and an interaction Hamiltonian describing the field-source interaction. In cases where the external source dynamics develops independently of our two-level atom dynamics in a prescribed manner, we just need to replace $\hat{\mathbf{D}}_{\text{free}}^{(+)}(\mathbf{0}, t)$ in (27.136) by the appropriate $\hat{\mathbf{D}}_{\text{ext}}^{(+)}(\mathbf{0}, t)$, i.e., $\tilde{a}_{qs}(0) \exp(-i\omega_q t)$ by $\tilde{a}_{qs}(t; \text{EXT})$.

The second term on the right side of (27.135) stems from the interaction of the atom with the radiative part of its own field, cf. (27.134). This interaction is quite complicated since it involves the solution of an integro-differential equation (in time), which furthermore is nonlinear because of the presence of the commutator between $\tilde{b}^\dagger(t)$ and $\tilde{b}(t)$. We will now make a dramatic simplification of the self-field interaction in two steps. Unless the mode frequency ω_q is extremely close to ω_0 , the exponential factor $\exp[i(\omega_q - \omega_0)(t' - t)]$ will vary rapidly in time (t') in comparison to $\tilde{b}(t')$ except for t' -values close to t . Disregarding the possible complications associated with resonant ($\omega_q \approx \omega_0$) modes, the main contribution to the time-integral thus comes from the time interval close to t . In case, it therefore is useful to make a Taylor series expansion of $\tilde{b}(t')$ around $t' = t$, i.e.,

$$\tilde{b}(t') = \tilde{b}(t) + (t' - t) \frac{d}{dt} \tilde{b}(t) + \dots \quad (27.137)$$

It appears from (27.135) that the first term in (27.137) gives a contribution to $d\tilde{b}(t)/dt$ proportional to g_{qs}^2 and the second term a contribution of the order g_{qs}^3 . By retaining only terms of order up to g_{qs}^2 we hence take $\tilde{b}(t') = \tilde{b}(t)$. This approximation removes the nonlocality of (27.135), and physically this means that the process now is memory-less. Such a process often is called a Markov process. It is quite interesting that the Markovian approximation indirectly removes the nonlinearity of the self-field. This is so because

$$[\tilde{b}^\dagger(t), \tilde{b}(t)] \tilde{b}(t) = -\tilde{b}(t). \quad (27.138)$$

The reader may prove this result by noting that (1) the anticommutator for the slowly varying operators $\tilde{b}^\dagger$ and $\tilde{b}$ is the same as for the rapidly varying ones ($\hat{b}^\dagger$ and $\hat{b}$), namely

$$\{\tilde{b}(t), \tilde{b}^\dagger(t)\} = \hat{1}, \quad (27.139)$$

and (2) $\tilde{b}^2 = 0$. In the first step we thus get

$$\left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \sum_{q,s} g_{qs}^2 \int_0^t \tilde{b}(t') e^{i(\omega_q - \omega_0)(t' - t)} \approx -\tilde{b}(t) \sum_{q,s} g_{qs}^2 \int_0^t e^{i(\omega_q - \omega_0)(t' - t)} dt'. \quad (27.140)$$

In the second step, we approximate the integral in (27.140) by the positive-frequency delta function (times 2π), that is

$$\begin{aligned} \int_0^t e^{i(\omega_q - \omega_0)(t' - t)} dt' &= \int_0^t e^{i(\omega_0 - \omega_q)\tau} d\tau \\ &\approx \lim_{t \rightarrow \infty} \int_0^t e^{i(\omega_0 - \omega_q)\tau} d\tau = 2\pi \delta^{(+)}(\omega_0 - \omega_q). \end{aligned} \quad (27.141)$$

We expect the approximation to hold for times $t \gg |\omega_0 - \omega_q|^{-1}$.

Together, the rotating-wave approximation, the Markovian approximation, and the $t \rightarrow \infty$ -approximation in (27.141), hence have resulted in the following result for the rate of change of the lowering operator:

$$\frac{d}{dt} \tilde{b}(t) = \tilde{R}_{\text{free}}(t) + \tilde{R}_{\text{spon}}(t) + \tilde{R}_{\text{Lamb}}(t), \quad (27.142)$$

where

$$\tilde{R}_{\text{free}}(t) = (i\hbar\epsilon_0)^{-1} e^{i\omega_0 t} \left[\tilde{b}^\dagger(t), \tilde{b}(t) \right] \mathbf{d}_{1 \rightarrow 2} \cdot \hat{\mathbf{D}}_{\text{free}}^{(+)}(\mathbf{0}, t), \quad (27.143)$$

$$\tilde{R}_{\text{spon}}(t) = -\pi \tilde{b}(t) \sum_{q,s} g_{qs}^2 \delta(\omega_0 - \omega_q), \quad (27.144)$$

and

$$\tilde{R}_{\text{Lamb}}(t) = i \tilde{b}(t) \sum_{q,s} g_{qs}^2 P \left(\frac{1}{\omega_0 - \omega_q} \right). \quad (27.145)$$

The last two terms in (27.142) are obtained by a division of positive-frequency delta function into its real and imaginary part; see (15.42).

27.6.3 The Spontaneous Decay Rate

The physical role of the term $\tilde{R}_{\text{spon}}(t)$ starts to appear after the summation over the field modes has been carried out. By using the expression for the coupling constant in (27.132), and by performing thereafter the summation over the polarization states for a given $\mathbf{q}$ via (15.52) one obtains

$$\begin{aligned}
\sum_{q,s} g_{qs}^2 \delta(\omega_q - \omega_0) &= \mathbf{d}_{1 \rightarrow 2} \cdot \left[\frac{1}{2\epsilon_0 \hbar L^3} \sum_{q,s} \omega_q \delta(\omega_0 - \omega_q) \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} \right] \cdot \mathbf{d}_{1 \rightarrow 2}^* \\
&= \mathbf{d}_{1 \rightarrow 2} \cdot \left[\frac{1}{2\epsilon_0 \hbar L^3} \sum_q \left(U - \frac{\mathbf{q} \cdot \mathbf{q}}{q^2} \right) \omega_q \delta(\omega_0 - \omega_q) \right] \cdot \mathbf{d}_{1 \rightarrow 2}^*.
\end{aligned} \tag{27.146}$$

If we now go to the continuum limit [relation (23.1)], and then make use of spherical coordinates with the polar axis along the $\mathbf{q}$ -direction, the angular integrations are easily carried out. Thus, we reach the result

$$\begin{aligned}
\sum_{q,s} g_{qs}^2 \delta(\omega_q - \omega_0) &= \frac{1}{2\epsilon_0 \hbar} \frac{|\mathbf{d}_{1 \rightarrow 2}|^2}{(2\pi)^2} \frac{4}{3} \int_0^\infty \left(\frac{\omega_q}{c_0} \right)^3 \delta(\omega_0 - \omega_q) d\left(\frac{\omega_q}{c_0} \right) \\
&= \frac{2}{3} \frac{|\mathbf{d}_{1 \rightarrow 2}|^2 \omega_0^3}{(2\pi)^2 \epsilon_0 \hbar c_0^3}.
\end{aligned} \tag{27.147}$$

The rate $\tilde{R}_{\text{spon}}(t)$ finally becomes

$$\tilde{R}_{\text{spon}}(t) = -\beta \tilde{b}(t), \tag{27.148}$$

where

$$\beta = \frac{2}{3} \frac{|\mathbf{d}_{1 \rightarrow 2}|^2 \omega_0^3}{4\pi \epsilon_0 \hbar c_0^3}. \tag{27.149}$$

If $\tilde{R}_{\text{spon}}(t)$ was the only term present on the right side of (27.141), the lowering operator would satisfy the equation

$$\frac{d}{dt} \tilde{b}(t) = -\beta \tilde{b}(t), \tag{27.150}$$

and the solution

$$\tilde{b}(t) = \tilde{b}(0) e^{-\beta t} \tag{27.151}$$

would tell us that $\tilde{b}(t)$ decays exponentially in time with a decay constant β . The quantity 2β is identical to the Einstein A-coefficient. In his famous derivation of Planck's radiation law, Einstein had to postulate that atoms can omit light spontaneously, i.e., without presence of any light field [324]. Einstein found that the rate of spontaneous photon emission must be $A = 2\beta$ in order to obtain agreement with Planck's law [367–370]. We shall soon see that the result in (27.151) contradicts quantum mechanics in a fundamental manner.

27.6.4 The Lamb-Shift Parameter

To obtain an explicit expression for $\tilde{R}_{\text{Lamb}}(t)$ in (27.145) we have to carry out the summation over the field modes. A comparison of (27.144) and (27.145) shows that the polarization-state summation and the angular integrations are identical for the $\tilde{R}_{\text{spont}}(t)$ and $\tilde{R}_{\text{Lamb}}$ calculations. With the replacement $\delta(\omega_0 - \omega_q) \Rightarrow (\pi i)^{-1} P [(\omega_0 - \omega_q)^{-1}]$ in the middle member of (27.147) one obtains

$$\tilde{R}_{\text{Lamb}}(t) = i\gamma \tilde{b}(t), \quad (27.152)$$

where

$$\gamma = \frac{2}{3} \frac{|\mathbf{d}_{1 \rightarrow 2}|^2}{4\pi^2 \epsilon_0 \hbar c_0^3} P \int_0^\infty \frac{\omega_q^3}{\omega_q - \omega_0} d\omega_q. \quad (27.153)$$

As it stands, the integral in (27.153) diverges. It must be remembered, however, that our analysis was limited to the interaction of the two-level atom with long-wavelength modes of the field. The upper limit of the integral should therefore be replaced by some finite value, but which? It is impossible to give a quantitative answer to this question within the theoretical framework used above. In a broader context, the problem of “infinities” was a nightmare for quantum electrodynamics in almost two decades after its birth. The gloom surrounding the infinity in $\gamma(\omega_0)$ began to vanish in 1947 when Bethe succeeded in calculating quite accurately the frequency split (Lamb shift) of the $2s_{1/2}$ and $2p_{1/2}$ states in hydrogen. Thus, Bethe obtained a value ≈ 1.040 MHz, in good agreement with experimental results obtained by Lamb and Retherford the same year. The present experimental value is ≈ 1.057 MHz. The relevant energy level diagram for the process is shown in Fig. 27.3.

Let me now briefly indicate how the problem of the infinite Lamb shift is solved. First of all, it is useful to return to the Coulomb gauge, and thus use the $\mathbf{p} \cdot \mathbf{A}$ -form of the interaction Hamiltonian. The matrix element of the momentum operator between the $|1\rangle$ and $|2\rangle$ -states then occurs, and the integrand $\omega_q^3/(\omega_q - \omega_0)$ is replaced by $\omega_q/(\omega_q - \omega_0)$. The principal value value integral still diverges, now linearly at high frequencies. Bethe pointed out that the divergence can mainly be associated with the electromagnetic mass of the electron. Let us for a moment go back to the “free-particle” Hamiltonian $p^2/(2m)$. Here, m is the experimentally observed mass. This mass inevitably includes the electron’s electromagnetic interaction with its own field (see Fig. 27.4), and the experimental mass deviates from the “bare” mass of the electron, m_{bare} , i.e., the mass the particle would have in the absence of the electromagnetic interaction. The difference between the two masses may be expressed in the form

$$\frac{1}{2m} = \frac{1}{2m_{\text{bare}}} - \Delta, \quad (27.154)$$

and a quantum electrodynamic calculation shows that the shift Δ is infinite! This, perhaps surprising result, is helpful, however, because it now is realized that the hitherto used “free-particle” Hamiltonian

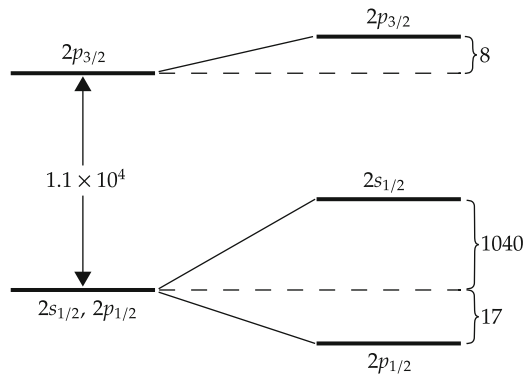


Fig. 27.3 Lamb shifts for the electron states with principal quantum number $n = 2$ in hydrogen. As usual, s and p denote the orbital angular momentum quantum number ($s : l = 0, p : l = 1$). In a relativistic calculation the position of the energy levels depend, besides on n , only on the total angular momentum $j = l + 1/2$ (indicated by the subscripts $1/2$ and $3/2$, here). According to the Dirac equation, the energy levels $2s_{1/2}$ and $2p_{1/2}$ should coincide (levels to the left). The radiative corrections split the $2s_{1/2}$ and $2p_{1/2}$ states, and lift the $2p_{3/2}$ state, as shown to the right in the figure. The numbers indicate the energy splits ($E/\hbar$) in MHz. In the nonrelativistic calculation of Bethe [327] only the position of the s -state is changed by the mass renormalization procedure

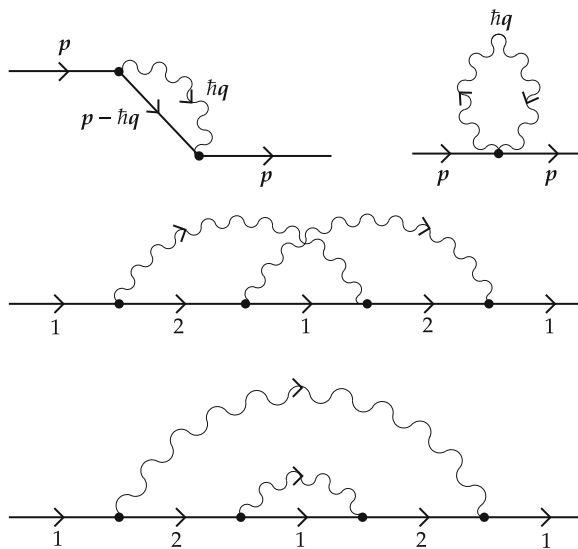


Fig. 27.4 Diagrammatic representation showing various radiative corrections to the self-energy (mass) of a free electron of momentum p . The two upper Feynman diagrams are for the second-order processes. *Left*: Two-step process where the electron (1) emits a photon with momentum $\hbar q$ and change momentum from p to $p - \hbar q$ ($p \cdot A$ -interaction) and (2) reabsorbs the photon and returns to momentum p ($p \cdot A$ -interaction). *Right*: One-step process with a simultaneous emission and reabsorption of the photon. The two lower Feynman diagrams show contributions to the electron self-energy in which virtual emission and reabsorption of two photons are involved

$$\frac{p^2}{2m} = \frac{p^2}{2m_{\text{bare}}} - ap^2 \quad (27.155)$$

contains a part $-ap^2$ which should be counted as a contribution to the interaction Hamiltonian. Hence, if one starts from the bare-mass kinetic energy $p^2/(2m_{\text{bare}})$ it is correct to use our familiar interaction Hamiltonian, H_I , but since we always begin with the observed kinetic energy $p^2/(2m)$, the correct Hamiltonian is $H_{\text{int}} + ap^2$. For many purposes the term ap^2 is unimportant, but for a correct prediction of Lamb shifts it is needed. When the ap^2 -term is included in the γ -calculation, one meets a principal integral of the form

$$I_\infty = P \int_0^\infty \omega_q \left(\frac{1}{\omega_q - \omega_0} - \frac{1}{\omega_q} \right) d\omega_q. \quad (27.156)$$

This integral is still divergent, but only logarithmically. In his nonrelativistic calculation, Bethe cut off the integral at the relativistic limit $\omega = mc_0^2/\hbar$ ($2mc_0^2$ is the electron-positron pair creation energy). Thus,

$$I_\infty \Rightarrow I = \omega_0 \ln \left(\frac{mc_0^2}{\hbar\omega_0} \right), \quad (27.157)$$

since $\hbar\omega_0 \ll mc_0^2$. The two-level approximation gives a poor estimate for the Lamb shift, and to come closer to reality one has to include all the atomic levels, as Bethe did. In a more sophisticated relativistic calculation the logarithmic divergence in (27.156) is not present, but the relevant relativistic integrand falls off rapidly at frequencies $\omega \gtrsim mc_0^2/\hbar$.

27.6.5 The Radiated Transverse Field

Let us now consider the radiation from a two-level atom initially placed in a photon vacuum. In Sect. 27.2.2, we studied the nonlocal relation between the transverse part of the vector potential and the flip operators. In the notation of lowering and raising operators (see (27.83) and (27.84)), (27.32) is reduced to the following form for a two-level atom:

$$\begin{aligned} \hat{A}_T(\mathbf{r}, t) = & \hat{A}_T^{\text{ext}}(\mathbf{r}, t) + \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{1}{|\mathbf{r} - \mathbf{r}'|} \left[\langle 2|\hat{\mathbf{J}}_T|1\rangle(\mathbf{r}', t_{\text{ret}}) \hat{b}^\dagger(t_{\text{ret}}) \right. \\ & \left. + \langle 1|\hat{\mathbf{J}}_T|2\rangle(\mathbf{r}', t_{\text{ret}}) \hat{b}(t_{\text{ret}}) \right] d^3r'. \end{aligned} \quad (27.158)$$

It is important for studies of correlation functions of the field, for instance, to know the positive- and negative-frequency components of $\hat{A}_T(\mathbf{r}, t)$. Since

$$\hat{A}_T^{(+)}(\mathbf{r}, t) = L^{-3/2} \sum_{q,s} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \hat{a}_{qs}(t) \epsilon_{qs} e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (27.159)$$

and $\hat{A}_T^{(-)}(\mathbf{r}, t) = (\hat{A}_T^{(+)}(\mathbf{r}, t))^\dagger$ it appears from (27.131) that $\hat{A}_T^{(+)}(\mathbf{r}, t)$ in the rotating-wave approximation used below relates to the term in (27.158) which contains $\hat{b}(t_{\text{ret}})$. For investigations of the spontaneous emission process we can also disregard the external vector potential (operator) since

$$\hat{A}_T^{(+)\text{ext}}(\mathbf{r}, t)|0\rangle = 0, \quad (27.160)$$

where $|0\rangle$ denotes the global vacuum state of the field. The result in (27.160) is obvious, remembering that the external field, here assumed to have been detached from its source, actually is a function of the various $\hat{a}_{qs}(0)$ -operators. With the remarks above one, therefore, may start the analysis of the spontaneous emission process from the effective operator relation

$$\hat{A}_T^{(+)}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\langle 1|\hat{\mathbf{J}}_T|2\rangle(\mathbf{r}', t_{\text{ret}})}{|\mathbf{r} - \mathbf{r}'|} \hat{b}(t_{\text{ret}}) d^3 r'. \quad (27.161)$$

As it stands, the matrix element $\langle 1|\hat{\mathbf{J}}_T|2\rangle$ depends on time. The reader may recall that this time dependence originates in the diamagnetic part of the current density operator, and that the corresponding matrix element usually is negligible, cf. the discussion in Sect. 27.2.3. The matrix element in (27.161) thus is replaced by its time independent paramagnetic part

$$\langle 1|\hat{\mathbf{J}}_T^0|2\rangle(\mathbf{r}) \equiv \int_{-\infty}^{\infty} \delta_T(\mathbf{r} - \mathbf{r}') \cdot \mathbf{j}_{2 \rightarrow 1}^0(\mathbf{r}') d^3 r', \quad (27.162)$$

where the expression for $\mathbf{j}_{2 \rightarrow 1}^0$ follows from (27.37). Hence, (27.161) is reduced to the form

$$\hat{A}_T^{(+)}(\mathbf{r}, t) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\langle 1|\hat{\mathbf{J}}_T^0|2\rangle(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \hat{b} \left(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0} \right) d^3 r'. \quad (27.163)$$

On the basis of certain approximations, we have seen that the slowly varying part of the lowering operator has a time evolution determined by (27.142). For application to spontaneous emission we can neglect the term $\tilde{R}_{\text{free}}(t)$, given by (27.143), because the free-field operator $\hat{\mathbf{D}}_{\text{free}}^{(+)}(\mathbf{0}, t)$ only is composed from field annihilation operators $\hat{a}_{qs}(0)$, see (27.136). With the last two terms on the right-hand-side of (27.142) given by (27.148) and (27.152) (with a finite γ) we thus have the following effective time-evolution equation for $\tilde{b}(t)$:

$$\frac{d}{dt} \tilde{b}(t) = (-\beta + i\gamma) \tilde{b}(t). \quad (27.164)$$

This equation immediately leads to the result

$$\hat{b}(t) = \hat{b}(0)e^{-\beta t}e^{-i(\omega_0 - \gamma)t}. \quad (27.165)$$

By utilizing (27.164), one obtains

$$\hat{A}_T^{(+)}(\mathbf{r}, t) = \mathcal{A}_T(\mathbf{r}, t)\hat{b}(0)e^{-\beta t}e^{-i(\omega_0 - \gamma)t}, \quad (27.166)$$

where

$$\begin{aligned} \mathcal{A}_T(\mathbf{r}, t) = & \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\langle 1 | \hat{\mathbf{J}}_T^0 | 2 \rangle(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ & \times \exp \left\{ [\beta + i(\omega_0 - \gamma)] \frac{|\mathbf{r} - \mathbf{r}'|}{c_0} \right\} \theta \left(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0} \right) d^3 r'. \end{aligned} \quad (27.167)$$

The result in (27.166) holds in the near-, mid- and far-field zones of the two-level atom. The atom starts its decay at $t = 0$, and the step function $\theta(t - |\mathbf{r} - \mathbf{r}'|/c_0)$ appearing in $\mathcal{A}_T(\mathbf{r}, t)$ ensures that the field operator $\hat{A}_T^{(+)}$ at the space-time point $(\mathbf{r}, t)$ only has (retarded) contributions from those regions of the transverse current density domain which satisfy the condition $t > |\mathbf{r} - \mathbf{r}'|/c_0$. For times so large that $t > R_{\max}/c_0$, where $R_{\max}$ is the maximum $|\mathbf{r} - \mathbf{r}'|$ -distance, the field operator at the observation point $\mathbf{r}$ will decay exponentially as a function of time (decay constant β) while oscillating with a frequency, $\omega_0 - \gamma$, slightly displaced from the transition frequency ω_0 .

For studies of second-order correlation effects of the spontaneously emitted electromagnetic field in various distances from the atom (also the rim zone), the mean value

$$\langle 0 | \hat{\mathbf{E}}_T^{(-)}(\mathbf{r}, t) \hat{\mathbf{E}}_T^{(+)}(\mathbf{r}, t + \tau) | 0 \rangle = \langle 0 | \frac{\partial \hat{A}_T^{(-)}(\mathbf{r}, t)}{\partial t} \frac{\partial \hat{A}_T^{(+)}(\mathbf{r}, t + \tau)}{\partial t} | 0 \rangle, \quad (27.168)$$

a dyadic quantity, is of particular relevance [53].

The frequency spectrum of the field operator $\hat{A}_T^{(+)}$ in (27.163) is obtained via a Fourier-integral transformation of the lowering operator, i.e.,

$$\begin{aligned} \int_{|\mathbf{r} - \mathbf{r}'|/c_0}^{\infty} \hat{b} \left(t - \frac{|\mathbf{r} - \mathbf{r}'|}{c_0} \right) e^{i\omega t} dt &= \exp \left(i \frac{\omega}{c_0} |\mathbf{r} - \mathbf{r}'| \right) \int_0^{\infty} \hat{b}(\tau) e^{i\omega\tau} d\tau \\ &= \exp \left(i \frac{\omega}{c_0} |\mathbf{r} - \mathbf{r}'| \right) \frac{\hat{b}(0)}{\beta - i(\omega - \omega_0 + \gamma)}. \end{aligned} \quad (27.169)$$

The lower limit on the first integral arises from the fact that $\hat{b}(\tau)$ is zero for $\tau < 0$, and the last member of (27.169) follows by use of (27.165). Hence, we obtain

$$\hat{A}_T^{(+)}(\mathbf{r}; \omega) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \frac{\langle 1 | \hat{\mathbf{J}}_T^0 | 2 \rangle(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \exp\left(i \frac{\omega}{c_0} |\mathbf{r} - \mathbf{r}'|\right) d^3 r' \frac{\hat{b}(0)}{\beta - i(\omega - \omega_0 + \gamma)}. \quad (27.170)$$

The spectral density [53] is obtained from (27.168) by taking the Fourier transform with respect to τ . For a single atom the correlation function and the spectral density both depend on the time t , so the radiation process is not stationary.

27.6.6 The $\{\hat{b}, \hat{b}^\dagger\}$ -Anticommutator Problem

The QED-description of the spontaneous decay forces us to incorporate dissipation effects in our quantum picture. To catch a glimpse of the quantum physical problem we are facing, let us assume that the Heisenberg operator $\hat{O}(t)$ and its Hermitian conjugate at time $t = 0$ satisfy the anticommutator relation

$$\{\hat{O}(0), \hat{O}^\dagger(0)\} = \hat{1}. \quad (27.171)$$

Since the operator $\hat{O}$ develops in time according to

$$\hat{O}(t) = e^{i\hat{H}t/\hbar} \hat{O}(0) e^{-i\hat{H}t/\hbar}, \quad (27.172)$$

where $\hat{H}$ is the total (time-independent) Hamilton operator of the system, it is easy to show that

$$\{\hat{O}(t), \hat{O}^\dagger(t)\} = \hat{1}. \quad (27.173)$$

The anti-commutation relation between $\hat{O}$ and $\hat{O}^\dagger$ thus is preserved over time. This fact also must hold for the lowering and raising operators which we know satisfy (27.88). For the *model* of spontaneous decay considered in the previous subsections, we reach the time dependence of $\hat{b}(t)$ given in (27.165). From this one obtains an anticommutator,

$$\{\hat{b}(t), \hat{b}^\dagger(t)\} = \{\hat{b}(0), \hat{b}^\dagger(0)\} e^{-2\beta t}, \quad (27.174)$$

which depends on time (and vanishes for $t \rightarrow \infty$).

In the present case it is possible to restore the fundamental criteria in (27.173) by taking into account the interaction of the two-level atom with the vacuum fluctuations in the electromagnetic field. The atom thus is subjected to damping and fluctuation forces, and altogether the anticommutator relation in (27.88) can be preserved over time, at least when averaged in a quantum-statistical sense over the fluctuations [303, 338]. The fluctuation-dissipation problem may be studied in a systematic manner using a density matrix formalism for the coupled atom-field system.

If one inserts the result $\tilde{b}(t) = \tilde{b}(0) \exp(-\beta + i\gamma)t$ into (27.134), it appears that

$$\tilde{a}_{qs}(t) = \tilde{a}_{qs}(0) + \eta(t)\tilde{b}(0), \quad (27.175)$$

where $\eta(t)$ is a time dependent c -number. Since the field and particle operators commute at $t = 0$, one obtains

$$[\tilde{a}_{qs}(t), \tilde{a}_{qs}^\dagger(t)] = [\tilde{a}_{qs}(0), \tilde{a}_{qs}^\dagger(0)] + |\eta(t)|^2 [\tilde{b}(0), \tilde{b}^\dagger(0)]. \quad (27.176)$$

As the reader may have anticipated, it is thus neither possible to maintain the fundamental commutator relation between the annihilation and creation operators of the field mode (23.46) over time.

With $\hat{b}(t)$ given by (27.165), the mean energy in the upper atomic level becomes as a function of time

$$\begin{aligned} \langle 2 | \hat{H}_A(t) | 2 \rangle &= \frac{1}{2} \hbar \omega_0 \langle 2 | \hat{b}^\dagger(t) \hat{b}(t) - \hat{b}(t) \hat{b}^\dagger(t) | 2 \rangle \\ &= \frac{1}{2} \hbar \omega_0 e^{-2\beta t} \langle 2 | \hat{b}^\dagger(0) \hat{b}(0) - \hat{b}(0) \hat{b}^\dagger(0) | 2 \rangle = \frac{1}{2} \hbar \omega_0 e^{-2\beta t}. \end{aligned} \quad (27.177)$$

The spontaneous decay process thus is exponential in time at a rate 2β .

27.6.7 Relation Between the Spontaneous Decay Rate and the Transverse Propagator

In (14.61) we gave the plane-wave eigenvector expansion of the transverse propagator over an infinite domain. If the expansion is over a finite domain, and we still use linearly polarized plane waves as eigenvectors, we obtain from (14.61)

$$G_T(\mathbf{r}_0, \mathbf{r}_0; \omega) = \frac{1}{L^3} \sum_{q,s} \frac{\epsilon_{qs} \epsilon_{qs}}{q^2 - q_0^2} = \frac{c_0^2}{L^3} \sum_q \frac{U - \kappa \kappa}{\omega_q^2 - \omega_0^2}. \quad (27.178)$$

To proceed we make use of the relation

$$P \int_{-\infty}^{\infty} \frac{F(\omega)}{\omega^2 - \omega_0^2} d\omega = \frac{\pi i}{2\omega_0} F(\omega_0) = \frac{\pi i}{2\omega_0} \int_{-\infty}^{\infty} F(\omega) \delta(\omega - \omega_0) d\omega. \quad (27.179)$$

The first part of (27.179) is proved by contour integration. The closed contour consists if a semicircle of infinite radius in the upper half-plane, and a contribution along the real axis. We assume that $F(\omega)$ decays so fast towards infinity that the integral along the semicircle gives zero. On the real axis we pass the pole at $\omega = \omega_0$ along a semicircle of infinitesimal small radius, as usual. By identifying the imaginary parts of (27.179) one obtains formally

$$P\left(\frac{\Im F(\omega)}{\omega^2 - \omega_0^2}\right) = \frac{\pi}{2\omega_0} \Re F(\omega) \delta(\omega - \omega_0). \quad (27.180)$$

Having in mind that the summation in (27.178) at the end of the calculation is to be replaced by an integral over $\mathbf{q}$ -space, we may write

$$\Im \mathbf{G}_T(\mathbf{r}_0, \mathbf{r}_0; \omega) = \frac{\pi c_0^2}{2\omega_0 L^3} \sum_{\mathbf{q}} (\mathbf{U} - \boldsymbol{\kappa} \boldsymbol{\kappa}) \delta(\omega_{\mathbf{q}} - \omega). \quad (27.181)$$

By a comparison of (27.146) and (27.181), it appears that the spontaneous decay rate can be written as follows:

$$\begin{aligned} \beta &= \pi \sum_{qs} g_{qs}^2 \delta(\omega_q - \omega_0) \\ &= \frac{\omega_0^2}{\epsilon_0 \hbar c_0^2} \mathbf{d}_{1 \rightarrow 2} \cdot \Im \mathbf{G}_T(\mathbf{r}_0, \mathbf{r}_0; \omega) \cdot \mathbf{d}_{1 \rightarrow 2}^*. \end{aligned} \quad (27.182)$$

Since we know that the imaginary part of the transverse propagator is given by $\mathbf{U} \omega_0 / (6\pi c_0)$ when the source and observation points coincide, (27.182) leads precisely back to the result in (27.149).

Chapter 28

Particle–Particle Interaction by Transverse Photon Exchange

In the Coulomb gauge formulation of quantum electrodynamics, elementary particles interact via two mechanisms: (1) An instantaneous Coulomb interaction and (2) a retarded interaction mediated by transverse photons. In the present chapter we shall study the electromagnetic interaction between just two particles (e.g., electrons) or composed particles (atoms, molecules, quantum dots, mesoscopic particles, etc.). In all cases, it is assumed that the probability density distributions of the two particles do not overlap in space. When composed particles come so close to each other that the tails of the density distributions begin to overlap electrons can move from one particle to the other by quantum mechanical tunneling, and if the distance is made sufficiently small one cannot in a meaningful manner treat the global system as a two-particle object.

We first consider the Coulomb interaction between the two particle systems, and we assume that the spatial extension of each of the two charge distributions is small in comparison to their separation. A multipole expansion of the interaction then shows that the leading term for two charged particle distributions has the form of a Coulomb interaction between point particles. For two neutral particles, which have nonvanishing electric dipole moments, the leading term has the character of a non-retarded dipole–dipole interaction.

In the fundamental case of two charged point particles the interaction mediated by transverse photons gives rise to a number of interesting physical phenomena. Here, we shall only discuss single-photon exchange in the limit where the energy of the photon is much larger than the typical Bohr transition energies. In this limit the photon exchange process can be described on the basis of a so-called effective electronic Hamiltonian acting essentially only in the particle state space. It appears from the analysis that the transverse photon exchange gives rise to delay and magnetic corrections to the Coulomb interaction.

We next show that the Van der Waals interaction between two neutral particles in the ground state, from the Power–Zienau–Woolley point of view, can be considered as an exchange process involving at least two transverse photons. When the distance between the particles is sufficiently small, the energies of the most important photons are much larger than the relevant Bohr energies. This again implies that an effective electronic Hamilton operator can be introduced. Second-order perturbation

theory in turn shows that the interaction energy between the particles is attractive, and varies with distance (R) as R^{-6} .

The Van der Waals interaction may also be of importance when a neutral particle (atom) is placed near a conducting surface. We briefly discuss this so-called Casimir effect in the case where the conductor is ideal and the particle is so close to the surface that field retardation effects can be neglected. Using image potential theory it is shown that the interaction energy varies with the particle distance R from the surface as R^{-3} . In consequence, the interaction force varies with R^{-4} . For a hydrogen atom in the ground state the interaction is attractive.

28.1 Multipole Expansion of the Coulomb Interaction Energy

Let us now return to the expression given in (9.64) for the instantaneous Coulomb energy of a system of particles characterized by the charge density $\rho(\mathbf{r}, t) \equiv \rho(\mathbf{r})$, and let us assume that the system consists of two always non-overlapping distributions $\rho_A(\mathbf{r})$ and $\rho_B(\mathbf{r})$. We refer to the A and B systems as particles, although the two subsystems may be those of single electrons, atoms, molecules, mesoscopic objects, etc. The Coulomb interaction energy between the A and B particles is given by

$$V_{\text{Coul}}^{\text{AB}} = \frac{1}{4\pi\epsilon_0} \int_{-\infty}^{\infty} \frac{\rho_A(\mathbf{r})\rho_B(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' d^3r, \quad (28.1)$$

and the spatial separation of A and B implies that $|\mathbf{r} - \mathbf{r}'| \neq 0$ for all pairs of space points, where ρ_A and ρ_B are nonvanishing. If we denote the center of mass coordinates for the two particles by $\mathbf{r}_A$ and $\mathbf{r}_B$, and the position coordinates measured relative to these by $\mathbf{\Delta}_A$ and $\mathbf{\Delta}_B$, i.e.,

$$\mathbf{r} = \mathbf{r}_A + \mathbf{\Delta}_A, \quad (28.2)$$

$$\mathbf{r}' = \mathbf{r}_B + \mathbf{\Delta}_B, \quad (28.3)$$

we have

$$\mathbf{r}' - \mathbf{r} = \mathbf{R} + \mathbf{\Delta}, \quad (28.4)$$

where $\mathbf{R} = \mathbf{r}_B - \mathbf{r}_A$, and $\mathbf{\Delta} = \mathbf{\Delta}_B - \mathbf{\Delta}_A$. In the following we assume that the spatial extension of each of the two charge distributions is small compared to their separation, i.e., $R = |\mathbf{r}_B - \mathbf{r}_A| \gg \Delta_A, \Delta_B$. With this assumption it is useful to expand the interaction energy in a certain multipole series. To this end, we start by a Taylor series expansion of $|\mathbf{r}' - \mathbf{r}|^{-1} = |\mathbf{R} + \mathbf{\Delta}|^{-1}$ around $\mathbf{R}$. Hence,

$$|\mathbf{r}' - \mathbf{r}|^{-1} = \frac{1}{R} - \frac{\hat{\mathbf{R}} \cdot \mathbf{\Delta}}{R^2} + \frac{1}{2R^3} \mathbf{\Delta} \cdot (3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U}) \cdot \mathbf{\Delta} + \dots, \quad (28.5)$$

where $\hat{\mathbf{R}} = \mathbf{R}/R$. Only the first three terms have been written out explicitly since no of the subsequent terms are needed below. I leave it as an exercise for the reader to prove in particular the correctness of the third term in (28.5). By inserting (28.5) into (28.1), one obtains an expansion,

$$V_{\text{Coul}}^{\text{AB}} = V_{(1)}^{\text{AB}} + V_{(2)}^{\text{AB}} + V_{(3)}^{\text{AB}} + \cdots, \quad (28.6)$$

in powers of the reciprocal center of mass distance, R^{-1} . The first term in (28.6), which is given by

$$V_{(1)}^{\text{AB}} = \frac{1}{4\pi\epsilon_0} \frac{q_A q_B}{R}, \quad (28.7)$$

where

$$q_I = \int_{-\infty}^{\infty} \rho_I(\mathbf{r}) d^3 r, \quad I = A, B, \quad (28.8)$$

is the charge of particle I, is just the usual Coulomb interaction energy between two point-particles. To calculate the second term in (28.6), we write $\mathbf{\Delta}$ in the form

$$\mathbf{\Delta} = \mathbf{r}' - \mathbf{r}_B - (\mathbf{r} - \mathbf{r}_A). \quad (28.9)$$

This, then gives

$$\begin{aligned} V_{(2)}^{\text{AB}} &= \frac{1}{4\pi\epsilon_0} R^{-2} \hat{\mathbf{R}} \cdot \left\{ \int_{-\infty}^{\infty} [\mathbf{r} - \mathbf{r}_A - (\mathbf{r}' - \mathbf{r}_B)] \rho_A(\mathbf{r}) \rho_B(\mathbf{r}') d^3 r' d^3 r \right\} \\ &= \frac{1}{4\pi\epsilon_0} \frac{(q_B \boldsymbol{\mu}_A - q_A \boldsymbol{\mu}_B) \cdot \hat{\mathbf{R}}}{R^2}, \end{aligned} \quad (28.10)$$

where

$$\boldsymbol{\mu}_I = \int_{-\infty}^{\infty} (\mathbf{r} - \mathbf{r}_I) \rho_I(\mathbf{r}) d^3 r \quad (28.11)$$

is the dipole moment of the charge distribution of particle I ($= A, B$) with respect to the center of mass. The contribution $V_{(2)}^{\text{AB}}$ hence represents the charge-dipole Coulomb interaction between the particles. This interaction will vanish unless at least one of the particles carries a net charge. Let us now consider the third term in the Coulomb interaction, viz.,

$$\begin{aligned} V_{(3)}^{\text{AB}} &= \frac{1}{4\pi\epsilon_0} \frac{1}{2R^3} \int_{-\infty}^{\infty} \rho_A(\mathbf{r}) \rho_B(\mathbf{r}) \\ &\quad \times \left\{ [\mathbf{r}' - \mathbf{r}_B - (\mathbf{r} - \mathbf{r}_A)] \cdot (3\hat{\mathbf{R}}\hat{\mathbf{R}} - \mathbf{U}) \cdot [\mathbf{r}' - \mathbf{r}_B - (\mathbf{r} - \mathbf{r}_A)] \right\} d^3 r' d^3 r. \end{aligned} \quad (28.12)$$

With the help of the tensorial quadrupole moment

$$\mathbf{Q}_I = \frac{1}{2} \int_{-\infty}^{\infty} \left[(\mathbf{r} - \mathbf{r}_I)(\mathbf{r} - \mathbf{r}_I) - \frac{1}{3} \mathbf{U}(\mathbf{r} - \mathbf{r}_I) \cdot (\mathbf{r} - \mathbf{r}_I) \right] \rho_I(\mathbf{r}) d^3 r, \quad (28.13)$$

which is a certain kind of second-order moment of the charge distribution of particle I (A, B) around its center of mass, and the vectorial dipole moment in (28.11), one may write $V_{(3)}^{AB}$ in the following form:

$$V_{(3)}^{AB} = \frac{1}{4\pi\epsilon_0} \frac{1}{R^3} \left[3\hat{\mathbf{R}} \cdot (q_B \mathbf{Q}_A + q_A \mathbf{Q}_B) \cdot \hat{\mathbf{R}} + \mu_A \cdot \mu_B - 3\hat{\mathbf{R}} \cdot \mu_A \mu_B \cdot \hat{\mathbf{R}} \right]. \quad (28.14)$$

The first part of (28.14) represents the instantaneous charge–quadrupole interaction between the particles. The second part, viz.,

$$\begin{aligned} V_{\text{dip-dip}}^{AB} &= \frac{1}{4\pi\epsilon_0} \frac{1}{R^3} \mu_A \cdot (U - 3\hat{\mathbf{R}}\hat{\mathbf{R}}) \cdot \mu_B \\ &= \epsilon_0^{-1} \mu_A \cdot \delta_L(R) \cdot \mu_B \end{aligned} \quad (28.15)$$

constitutes the non-retarded dipole–dipole interaction energy, and for neutral particles $V_{\text{dip-dip}}^{AB}$ usually is the leading term in the Coulomb interaction. The dipole–dipole coupling is effective only among particles in near-field contact, and it relates to the so-called Van der Waals interaction in a manner to be discussed in Sect. 28.4. If μ_A , μ_B and $\hat{\mathbf{R}}$ are mutually orthogonal the dipole–dipole coupling vanishes.

28.2 Perturbation by an Effective Electronic Hamiltonian

In Sect. 28.3, we shall briefly discuss how the Coulomb interaction between two charged particles is modified by the exchange of transverse photons, and in Sect. 28.4 we shall argue that the Van der Waals interaction between two neutral atoms may be considered as originating in the exchange of pairs of transverse photons. For a qualitative understanding of the two types of interaction we shall find it useful to subject the total Hamiltonian of the particle field system to a certain kind of unitary transformation. If the energies of the transverse photons are sufficiently large, the new Hamiltonian appears as an effective Hamiltonian acting only in the particle subspace. In a sense one may thus “forget” that it is the electromagnetic field which is responsible for the interaction between the two particles. In the present section we shall introduce the unitary transformation which in the end leads us to the effective electronic interaction Hamiltonian.

Let us start by a division of the global particle–field Hamiltonian, $\hat{H}$, into two parts, i.e.,

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}, \quad (28.16)$$

where $\hat{H}_0$ is the Hamiltonian one would have in the absence of coupling between the particles and the field, and $\hat{V}$ is the interaction Hamiltonian. To keep track of the various orders of interaction in a perturbation calculation, we have as usual multiplied $\hat{V}$ by a dimensionless parameter λ [$|\lambda| < 1$], which by the end of the calculation is

set to one. The eigenstates of $\hat{H}_0$, $|i; \alpha\rangle$, are tensor products of the particle, $|i\rangle$, and global field, $|\alpha\rangle$, eigenstates:

$$|i; \alpha\rangle = |i\rangle \otimes |\alpha\rangle. \quad (28.17)$$

In the following, particle states are characterized by Roman letters such as i , and field states by Greek letters such as α . The eigenvalue equation for $\hat{H}_0$ is

$$\hat{H}_0|i; \alpha\rangle = (E_i + E_\alpha)|i; \alpha\rangle \equiv E_{i\alpha}|i; \alpha\rangle \quad (28.18)$$

where E_i and E_α are the eigenenergies of the particle system and the field.

The unitary transformation

$$\hat{T} = e^{i\hat{S}}, \quad (28.19)$$

with

$$\hat{S} = \hat{S}^\dagger, \quad (28.20)$$

transforms the global Hamiltonian into

$$\hat{H}' = \hat{T} \hat{H} \hat{T}^\dagger. \quad (28.21)$$

By means of the operator expansion theorem (25.115), we thus have the expansion

$$\hat{H}' = \hat{H} + [\hat{i}\hat{S}, \hat{H}] + \frac{1}{2!}[\hat{i}\hat{S}, [\hat{i}\hat{S}, \hat{H}]] + \cdots. \quad (28.22)$$

To determine the relevant $\hat{S}$ for the present purpose, it is convenient to expand $\hat{S}$ in a power series in λ ,

$$\hat{S} = \lambda\hat{S}_1 + \lambda^2\hat{S}_2 + \cdots. \quad (28.23)$$

Since we just want $\hat{T}$ to change the interaction Hamiltonian, no zero-order term in λ is included in (28.23). By inserting (28.16) and (28.23) into (28.22) we obtain an expansion

$$\hat{H}' = \hat{H}_0 + \lambda\hat{H}'_1 + \lambda^2\hat{H}'_2 + \cdots \quad (28.24)$$

for which the explicit forms of the first- and second-order terms in λ are

$$\lambda\hat{H}'_1 = [i\lambda\hat{S}_1, \hat{H}_0] + \lambda\hat{V}, \quad (28.25)$$

and

$$\lambda^2\hat{H}'_2 = [i\lambda^2\hat{S}_2, \hat{H}_0] + [i\lambda\hat{S}_1, \lambda\hat{V}] + \frac{1}{2}[i\lambda\hat{S}_1, [i\lambda\hat{S}_1, \hat{H}_0]]. \quad (28.26)$$

It is not difficult to write down the general expression for $\lambda^n \hat{H}'_n$, but in what follows we only need the terms for $n = 1, 2$.

We now require that $\hat{H}'$ and $\hat{S}$ satisfy the operator requirements

$$\hat{P}_\alpha \hat{H}' \hat{P}_\beta = 0, \quad \alpha \neq \beta, \quad (28.27)$$

and

$$\hat{P}_\alpha \hat{S} \hat{P}_\alpha = 0, \quad \forall \alpha, \quad (28.28)$$

where

$$\hat{P}_\alpha = \sum_i |i; \alpha\rangle \langle i; \alpha| = |\alpha\rangle \langle \alpha| \quad (28.29)$$

is the projector over the α -manifold. The conditions in (28.27) and (28.28) allow one to determine the terms in $\hat{S}$ (28.23) step by step, as I now shall indicate. From the identity

$$\hat{P}_\alpha \hat{H}' \hat{P}_\beta = \sum_{i,j} |i; \alpha\rangle \langle i; \alpha| \hat{H}' |j; \beta\rangle \langle j; \beta| \quad (28.30)$$

it appears that the condition in (28.27) is tantamount to the requirement

$$\langle i; \alpha | \hat{H}' | j; \beta \rangle = 0, \quad \alpha \neq \beta, \quad (28.31)$$

which in turn, via (28.25), gives

$$\langle i; \alpha | [i \lambda \hat{S}_1, \hat{H}_0] | j; \beta \rangle + \langle i; \alpha | \lambda \hat{V} | j; \beta \rangle = 0 \quad (28.32)$$

for $\alpha \neq \beta$. By utilizing the eigenvalue equation for $\hat{H}_0$, one obtains the following relation between the matrix elements of $\hat{S}_1$ and $\hat{V}$:

$$\langle i; \alpha | i \lambda \hat{S}_1 | j; \beta \rangle = \frac{\langle i; \alpha | \lambda \hat{V} | j; \beta \rangle}{E_{i\alpha} - E_{j\beta}}, \quad \alpha \neq \beta. \quad (28.33)$$

Since

$$\hat{P}_\alpha \hat{S} \hat{P}_\alpha = \sum_{i,j} |i; \alpha\rangle \langle i; \alpha | \hat{S} | j; \alpha\rangle \langle j; \alpha| \quad (28.34)$$

it is obvious that the requirement in (28.28) leads to

$$\langle i; \alpha | i \lambda \hat{S}_1 | j; \alpha \rangle = 0, \quad \forall \alpha. \quad (28.35)$$

Together, (28.33) and (28.35) thus determine all the matrix elements of $\hat{S}_1$ for a given interaction Hamiltonian, $\hat{V}$. We know from the requirement in (28.31) that the first-order operator $\lambda \hat{H}'_1$ has nonvanishing matrix elements only within a given α -manifold, and by utilizing (28.35) it appears from (28.25) that these matrix elements are given by

$$\langle i; \alpha | \lambda \hat{H}'_1 | j; \alpha \rangle = \langle i; \alpha | \lambda \hat{V} | j; \alpha \rangle, \quad \forall \alpha. \quad (28.36)$$

Let us now turn the attention towards the second-order operator $\lambda^2 \hat{H}'_2$, which of course also only has nonvanishing matrix elements within the α -manifold because of the general requirement in (28.31). From (28.26) we obtain

$$\begin{aligned} \langle i; \alpha | \lambda^2 \hat{H}'_2 | j; \alpha \rangle &= \langle i; \alpha | [i \lambda^2 \hat{S}_2, \hat{H}_0] | j; \alpha \rangle \\ &+ \langle i; \alpha | [i \lambda \hat{S}_1, \lambda \hat{V} + \frac{1}{2} [i \lambda \hat{S}_1, \hat{H}_0]] | j; \alpha \rangle. \end{aligned} \quad (28.37)$$

The first term on the right side of (28.37) is zero due to the requirement in (28.28). Thus,

$$\langle i; \alpha | [i \lambda^2 \hat{S}_2, \hat{H}_0] | j; \alpha \rangle = (E_{j\alpha} - E_{i\alpha}) \langle i; \alpha | i \lambda^2 \hat{S}_2 | j; \alpha \rangle = 0. \quad (28.38)$$

The second term can, with the help of (28.25), be rewritten in the form

$$\begin{aligned} &\langle i; \alpha | [i \lambda \hat{S}_1, \lambda \hat{V} + \frac{1}{2} [i \lambda \hat{S}_1, \hat{H}_0]] | j; \alpha \rangle \\ &= \langle i; \alpha | [i \lambda \hat{S}_1, \frac{1}{2} \lambda \hat{V}] | j; \alpha \rangle + \frac{1}{2} \langle i; \alpha | [i \lambda \hat{S}_1, \lambda \hat{H}'_1] | j; \alpha \rangle. \end{aligned} \quad (28.39)$$

The last matrix element in this equation vanishes as a result of the requirements in (28.27) and (28.28). To prove this assertion, one just inserts the completeness relation

$$\sum_{k, \gamma} |k; \gamma\rangle \langle k; \gamma| = \hat{1} \quad (28.40)$$

between the operators $\hat{S}_1$ and $\hat{H}'_1$. Hence,

$$\begin{aligned} \langle i; \alpha | [i \lambda \hat{S}_1, \lambda \hat{H}'_1] | j; \alpha \rangle &= \sum_{k, \gamma} \left(\langle i; \alpha | i \lambda \hat{S}_1 | k; \gamma \rangle \langle k; \gamma | \lambda \hat{H}'_1 | j; \alpha \rangle \right. \\ &\left. - \langle i; \alpha | \lambda \hat{H}'_1 | k; \gamma \rangle \langle k; \gamma | i \lambda \hat{S}_1 | j; \alpha \rangle \right) = 0, \end{aligned} \quad (28.41)$$

due to the fact that the matrix elements of $\lambda \hat{H}'_1$ vanish unless $\gamma = \alpha$. For $\gamma = \alpha$ we are left with matrix elements of $\alpha \hat{S}_1$ between states within the α -manifold. These matrix elements are zero. Altogether, it appears from (28.37), (28.38) and (28.41) that the matrix elements of $\lambda^2 \hat{H}'_2$ within the α -manifold are given by

$$\langle i; \alpha | \lambda^2 \hat{H}'_2 | j; \alpha \rangle = \frac{1}{2} \langle i; \alpha | [i \lambda \hat{S}_1, \lambda \hat{V}] | j; \alpha \rangle. \quad (28.42)$$

By now we only need to eliminate $i \lambda \hat{S}$ in favor of $\lambda \hat{V}$. This is done by means of (28.33), (28.35) and the completeness relation in (28.40).

$$\begin{aligned}
\langle i; \alpha | \lambda^2 \hat{H}'_2 | j; \alpha \rangle &= \frac{1}{2} \sum_{k, \gamma \neq \alpha} \left(\langle i; \alpha | i \lambda \hat{S}_1 | k; \gamma \rangle \langle k; \gamma | \lambda \hat{V} | j; \alpha \rangle \right. \\
&\quad \left. - \langle i; \alpha | \lambda \hat{V} | k; \gamma \rangle \langle k; \gamma | i \lambda \hat{S}_1 | j; \alpha \rangle \right) \\
&= \frac{1}{2} \sum_{k, \gamma \neq \alpha} \left(\frac{1}{E_{i\alpha} - E_{k\gamma}} + \frac{1}{E_{j\alpha} - E_{k\gamma}} \right) \\
&\quad \langle i; \alpha | \lambda \hat{V} | k; \gamma \rangle \langle k; \gamma | \lambda \hat{V} | j; \alpha \rangle.
\end{aligned} \tag{28.43}$$

By now, there is no need for the λ -parameter, and with $\lambda = 1$, it follows from (28.24), (28.36) and (28.43) that the transformed Hamiltonian to second order in $\hat{V}$ has the following three matrix elements within the α -manifold:

$$\begin{aligned}
\langle i; \alpha | \hat{H}' | j; \alpha \rangle &= E_{i\alpha} \delta_{ij} + \langle i; \alpha | \hat{V} | j; \alpha \rangle \\
&= \frac{1}{2} \sum_{k, \gamma \neq \alpha} \left(\frac{1}{E_{i\alpha} - E_{k\gamma}} + \frac{1}{E_{j\alpha} - E_{k\gamma}} \right) \langle i; \alpha | \hat{V} | k; \gamma \rangle \langle k; \gamma | \hat{V} | j; \alpha \rangle.
\end{aligned} \tag{28.44}$$

The first term of (28.44) relates to the unperturbed eigenenergies of the states within the α -manifold, and the second term represents the direct coupling energy between the different levels (here i and j) within the given α -manifold. The third term represents the indirect coupling between the i and j states in the α -manifold. This coupling goes through all levels ($k; \gamma$) of all other ($\gamma \neq \alpha$) manifolds. In their structure the terms of (28.44) resemble those of ordinary perturbation theory. Thus, for $i = j$ one obtains “almost” the standard result for the energy correction of state $|i; \alpha\rangle$: One must just remember that the second-order correction to the mean value $\langle i; \alpha | \hat{H}' | i; \alpha \rangle$ has no contributions from the states in the α -manifold.

28.3 Single-Photon Exchange Between Two Charged Particles

In this section, we shall briefly discuss how the Coulomb interaction energy between two charged particles (28.7) is modified by the exchange of transverse photons. We shall not carry out a general calculation but rather focus the attention on a certain limit in which the interaction between the particles can be described by a high-frequency approximation to the effective particle (electronic) Hamiltonian introduced in Sect. 28.2. We further restrict our considerations to a second-order perturbation theory (28.44) for which only exchange of single transverse photons exists. The analysis leads to two first-order corrections to the Coulomb interaction: (1) A delay correction to the Coulomb energy, and (2) a magnetic interaction energy associated with the particle velocities. Although the final result is identical to that obtained in the classical theory, the physics of the interaction process is seen in a

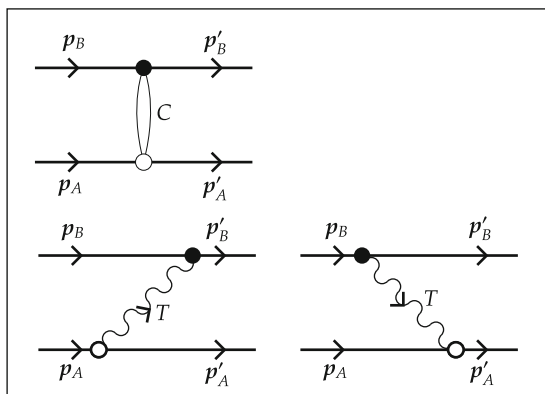


Fig. 28.1 Feynman diagrams illustrating part of the electromagnetic interaction between two charged particles (A and B) initially in the momentum states $|p_A\rangle$ and $|p_B\rangle$. The particles are scattered into the final states $|p'_A\rangle$ and $|p'_B\rangle$ by three processes: (1) Coulomb interaction (*top figure*), (2) emission of a transverse photon by A and reabsorption of this photon by B (*bottom figure to the left*), and (3) transverse photon emission from B and reabsorption in A (*bottom figure to the right*). The two single-photon exchange processes give a first correction to the Coulomb interaction energy between the particles

new perspective. A schematic illustration of the electromagnetic interaction between the two charged particles is shown in Fig. 28.1.

28.3.1 Qualitative Analysis of the Effective Hamiltonian to Second Order

For two particles (A and B) with masses (m_A, m_B) and charges (q_A, q_B) the Hamilton operator of the coupled particle–field system in the Coulomb gauge is given by (see (23.83))

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \quad (28.45)$$

where we as the unperturbed Hamiltonian have taken that of the free particles and the free field, i.e.,

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}_A^2}{2m_A} + \frac{\hat{\mathbf{p}}_B^2}{2m_B} + \hat{H}_F. \quad (28.46)$$

With this choice the Coulomb interaction energy is included in the interaction Hamiltonian. Thus,

$$\begin{aligned} \hat{H}_I = & \frac{1}{4\pi\epsilon_0} \frac{q_A q_B}{|\mathbf{r}_A - \mathbf{r}_B|} + \frac{q_A^2}{2m_A} \hat{\mathbf{A}}_T^2(\mathbf{r}_A) + \frac{q_B^2}{2m_B} \hat{\mathbf{A}}_T^2(\mathbf{r}_B) \\ & - \frac{q_A}{m_A} \hat{\mathbf{p}}_A \cdot \hat{\mathbf{A}}_T(\mathbf{r}_A) - \frac{q_B}{m_B} \hat{\mathbf{p}}_B \cdot \hat{\mathbf{A}}_T(\mathbf{r}_B), \end{aligned} \quad (28.47)$$

neglecting the Coulomb self-energy of the particles. In the context of the effective electronic Hamilton formalism established in Sect. 28.2, hence we start from $\hat{V} = \hat{H}_I$ in the second-order expression given in (28.44) for the matrix elements of the transformed Hamiltonian within the α -manifold. Let us now describe the various physical processes which are contained in the framework of (28.44) and (28.47).

Coulomb Interaction

The Coulomb interaction Hamiltonian, given by the first term on the right side of (28.47), contains only particle operators ($\mathbf{r}_A, \mathbf{r}_B$), and therefore it cannot connect states with different photon numbers. This implies that the Coulomb interaction Hamiltonian only contributes to the first-order term, $\langle i; \alpha | \hat{V} | j; \alpha \rangle$, in (28.44). Not only does its contribution of second order vanish, all higher-order perturbation terms are also zero, as the reader might have anticipated. In the nonretarded limit ($c_0 \rightarrow \infty$), the Coulomb interaction Hamiltonian (28.7) alone is responsible for the coupling between the two charged particles. In elementary quantum mechanics studies of two-particle scattering problems (and calculations of bound stationary states of two-particle systems) are most often based on the nonretarded Coulomb interaction approximation. The independence of the Coulomb interaction on the state of the field may be emphasized by the relation

$$\langle i; \alpha | |\mathbf{r}_A - \mathbf{r}_B|^{-1} | j; \alpha \rangle = \langle i | |\mathbf{r}_A - \mathbf{r}_B|^{-1} | j \rangle, \quad (28.48)$$

which clearly holds for the tensor product states in (28.17), assuming the global field state is normalized, $\langle \alpha | \alpha \rangle = 1$.

The $A_T \cdot A_T$ -Interaction

The charges q_A and q_B appear as coupling parameters, and working in lowest order we only keep terms proportional to q_A^2 , q_B^2 , and $q_A q_B$. The two terms in (28.47) which contain an $\hat{A}_T \cdot \hat{A}_T$ -factor therefore cannot contribute to the particle-particle interaction. They do affect the electrodynamics of each of the two particles, however. For particle A we thus obtain for the term proportional to $\hat{V}$ in (28.44)

$$\frac{q_A^2}{2m_A} \langle i; \alpha | \hat{A}_T^2(\mathbf{r}_A) | j; \alpha \rangle = \delta_{ij} \frac{q_A^2}{2m_A} \langle \alpha | \hat{A}_T^2(\mathbf{r}_A) | \alpha \rangle. \quad (28.49)$$

To determine the mean value of $\hat{A}_T^2(\mathbf{r}_A)$ in the global photon state $|\alpha\rangle$ we utilize the plane-wave expansion of $\hat{A}_T(\mathbf{r}_A)$ (23.47). Since a product of two field operators belonging to different modes cannot contribute to the mean value, one immediately gets

$$\begin{aligned}
\langle \alpha | \hat{A}_T^2(\mathbf{r}_A) | \alpha \rangle &= L^{-3} \sum_{q,s} \frac{\hbar}{2\epsilon_0 \omega_q} \langle \alpha | \hat{a}_{qs} \hat{a}_{qs}^\dagger + \hat{a}_{qs}^\dagger \hat{a}_{qs} | \alpha \rangle \\
&= L^{-3} \sum_{q,s} \frac{\hbar}{\epsilon_0 \omega_q} \left(N_{qs}^\alpha + \frac{1}{2} \right), \tag{28.50}
\end{aligned}$$

where for the $|\alpha\rangle$ -state, N_{qs}^α is the number of photons in the mode $(\mathbf{q}, s)$. By inserting the result above into (28.49) we obtain

$$\frac{q_A^2}{2m_A} \langle i; \alpha | \hat{A}_T^2(\mathbf{r}_A) | j; \alpha \rangle = \delta_{ij} L^{-3} \sum_{q,s} \frac{\hbar q_A^2}{2m_A \epsilon_0 \omega_q} \left(N_{qs}^\alpha + \frac{1}{2} \right). \tag{28.51}$$

The quantity

$$\Delta E_{12}^A = \frac{\hbar q_A^2}{2m_A \epsilon_0 L^3} \sum_q \omega_q^{-1} \tag{28.52}$$

represents the vibrational kinetic energy of particle A in the vacuum fluctuations, and with this energy is associated a radiative mass correction to m_A .

The $\mathbf{p} \cdot \mathbf{A}_T$ -Interaction

Let us turn our attention towards the role of the two last terms in (28.47). Since the transverse vector potential operator is linear in the mode annihilation and creation operators it is clear that these terms cannot contribute to the effective Hamiltonian in first-order perturbation theory. In second order we meet four types of processes:

$$\begin{aligned}
\langle i; \alpha | \hat{V} | k; \gamma \rangle \langle k; \gamma | \hat{V} | j; \alpha \rangle &= \sum_{I=A,B} \frac{q_I^2}{m_I^2} \langle i; \alpha | \hat{\mathbf{p}}_I \cdot \hat{\mathbf{A}}_T(\mathbf{r}_I) | k; \gamma \rangle \langle k; \gamma | \hat{\mathbf{p}}_I \cdot \hat{\mathbf{A}}_T(\mathbf{r}_I) | j; \alpha \rangle \\
&+ \frac{q_A q_B}{m_A m_B} \langle i; \alpha | \hat{\mathbf{p}}_A \cdot \hat{\mathbf{A}}_T(\mathbf{r}_A) | k; \gamma \rangle \langle k; \gamma | \hat{\mathbf{p}}_B \cdot \hat{\mathbf{A}}_T(\mathbf{r}_B) | j; \alpha \rangle \\
&+ (A \leftrightarrow B), \tag{28.53}
\end{aligned}$$

where the fourth term, $(A \leftrightarrow B)$, is obtained from the third term by interchange of the indices A and B. It is these two last terms which are responsible for the particle–particle interaction by photon exchange. The first two terms describe processes in which particle A (B) (1) emits and reabsorbs a photon, or (2) absorbs and reemits a photon. For an electromagnetic field initially in a vacuum state $(|0\rangle)$ only the processes (1) can occur.

Consider now the situation where two free particles, initially with respective momenta $\mathbf{p}_A$ and $\mathbf{p}_B$, are scattered into the states $\mathbf{p}'_A$ and $\mathbf{p}'_B$ by photon exchange and let us for simplicity assume that the radiation field before and after the scattering process is in its global vacuum state. The state vectors of the initial (i) and final (f) states thus are

$$|\psi_i\rangle = |\mathbf{p}_A, \mathbf{p}_B; 0\rangle = |\mathbf{p}_A, \mathbf{p}_B\rangle \otimes |0\rangle = |\mathbf{p}_A\rangle \otimes |\mathbf{p}_B\rangle \otimes |0\rangle, \tag{28.54}$$

and

$$|\psi_f\rangle = |\mathbf{p}'_A, \mathbf{p}'_B; 0\rangle = |\mathbf{p}'_A, \mathbf{p}'_B\rangle \otimes |0\rangle = |\mathbf{p}'_A\rangle \otimes |\mathbf{p}'_B\rangle \otimes |0\rangle, \quad (28.55)$$

respectively. It is obvious from (28.53) that the intermediate field state must be a one-photon state, i.e., $|\gamma\rangle = |\mathbf{q}s\rangle$. For such a state we have

$$\langle 0|\hat{\mathbf{A}}_T(\mathbf{r}_A)|\mathbf{q}s\rangle\langle\mathbf{q}s|\hat{\mathbf{A}}_T(\mathbf{r}_B)|0\rangle = \frac{1}{L^3} \frac{\hbar}{2\epsilon_0\omega_q} \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} e^{i\mathbf{q}\cdot(\mathbf{r}_A - \mathbf{r}_B)}. \quad (28.56)$$

The parts of (28.53) which relate to the photon exchange process therefore are reduced to

$$\begin{aligned} & \langle \mathbf{p}'_A, \mathbf{p}'_B; 0 | \hat{V} | \mathbf{p}''_A, \mathbf{p}''_B; \mathbf{q}s \rangle \langle \mathbf{p}'_A, \mathbf{p}'_B; \mathbf{q}s | \hat{V} | \mathbf{p}_A, \mathbf{p}_B; 0 \rangle_{\text{EXCHANGE}} \\ &= \frac{q_A q_B}{m_A m_B} \frac{1}{L^3} \frac{\hbar}{2\epsilon_0\omega_q} \langle \mathbf{p}'_A, \mathbf{p}'_B | \hat{\mathbf{p}}_A \cdot \boldsymbol{\epsilon}_{qs} e^{i\mathbf{q}\cdot\mathbf{r}_A} | \mathbf{p}''_A, \mathbf{p}''_B \rangle \\ & \langle \mathbf{p}''_A, \mathbf{p}''_B | \hat{\mathbf{p}}_B \cdot \boldsymbol{\epsilon}_{qs} e^{-i\mathbf{q}\cdot\mathbf{r}_B} | \mathbf{p}_A, \mathbf{p}_B \rangle + (A \leftrightarrow B), \end{aligned} \quad (28.57)$$

where the matrix elements are taken in the particle subspace.

In the initial state the two particles together have the energy

$$E_{\text{par}} = \frac{\mathbf{p}_A^2}{2m_A} + \frac{\mathbf{p}_B^2}{2m_B}. \quad (28.58)$$

This energy also is the total energy of the global particle-field system since there are no photons to begin with. If we denote the energies of the particles in the intermediate and final states by E''_{par} and E'_{par} , and remember that the intermediate state contains just one photon, the parenthesis behind the summation sign in (28.44) is given by

$$\frac{1}{E_{i\alpha} - E_{k\alpha}} + \frac{1}{E_{j\alpha} - E_{k\alpha}} = \frac{1}{E_{\text{par}} - E''_{\text{par}} - \hbar\omega_q} + \frac{1}{E'_{\text{par}} - E''_{\text{par}} - \hbar\omega_q} \quad (28.59)$$

in a transition to the intermediate photon state $|\mathbf{q}s\rangle$. If the Bohr transition frequencies in (28.59) are small in comparison to all relevant frequencies, i.e.,

$$\frac{|E_{\text{par}} - E''_{\text{par}}|}{\hbar}, \frac{|E'_{\text{par}} - E''_{\text{par}}|}{\hbar} \ll \omega_q, \quad (28.60)$$

the right side of (28.59) equals in a first approximation $-2/(\hbar\omega_q)$. Apart from a few remarks, to be given in relation to a discussion of the momentum exchange (Sect. 28.3.3), we shall not analyze under which conditions the inequalities in (28.60) are satisfied. By neglect of the Bohr transition frequencies, an interesting approximate description of the photon exchange process emerges, as we shall see now.

By inserting (28.57) into (28.44), it appears that the matrix element of relevance for the photon exchange process becomes

$$\begin{aligned}
 & \langle p'_A, p'_B; 0 | \hat{H}'_2 | p_A, p_B; 0 \rangle_{\text{EXCHANGE}} \\
 &= - \sum_{q,s} \sum_{p''_A, p''_B} \frac{1}{2\epsilon_0 L^3} \frac{q_A q_B}{m_A m_B} \frac{1}{\omega_q^2} \\
 & \quad \times \langle p'_A, p'_B | \hat{p}_A \cdot \epsilon_{qs} e^{i q \cdot r_A} | p''_A, p''_B \rangle \langle p''_A, p''_B | \hat{p}_B \cdot \epsilon_{qs} e^{-i q \cdot r_B} | p_A, p_B \rangle \\
 & \quad + (A \leftrightarrow B). \tag{28.61}
 \end{aligned}$$

The intermediate particle states can be eliminated from (28.61) by use of the closure theorem in the particle subspace, viz.,

$$\sum_{p''_A, p''_B} | p''_A, p''_B \rangle \langle p''_A, p''_B | = \hat{1}, \tag{28.62}$$

giving,

$$\begin{aligned}
 & \langle p'_A, p'_B; 0 | \hat{H}'_2 | p_A, p_B; 0 \rangle_{\text{EXCHANGE}} = - \frac{1}{2\epsilon_0 L^3} \frac{q_A q_B}{m_A m_B} \sum_{q,s} \frac{1}{\omega_q^2} \\
 & \quad \times \langle p'_A, p'_B | \hat{p}_A \cdot \epsilon_{qs} \epsilon_{qs} \cdot \hat{p}_B e^{i q \cdot (r_A - r_B)} | p_A, p_B \rangle + (A \leftrightarrow B). \tag{28.63}
 \end{aligned}$$

It appears from the foregoing calculation that, in the certain approximation for which the Bohr frequencies are negligible, the matrix element of relevance for the photon exchange process is given by

$$\langle p'_A, p'_B; 0 | \hat{H}'_2 | p_A, p_B; 0 \rangle_{\text{EXCHANGE}} = \langle p'_A, p'_B | \hat{H}_2^{\text{eff}} | p_A, p_B \rangle, \tag{28.64}$$

where

$$\hat{H}_2^{\text{eff}} = - \frac{1}{2\epsilon_0 L^3} \frac{q_A q_B}{m_A m_B} \sum_{q,s} \frac{1}{\omega_q^2} \hat{p}_A \cdot \epsilon_{qs} \epsilon_{qs} \cdot \hat{p}_B e^{i q \cdot (r_A - r_B)} + (A \leftrightarrow B) \tag{28.65}$$

is an effective particle Hamiltonian acting only in the particle subspace. Such an effective particle Hamiltonian could have been introduced for the single-photon exchange process without making the approximations in (28.60). If one in the “A ↔ B”-part of (28.65) makes the substitution $\mathbf{q} \rightarrow -\mathbf{q}$, it is not difficult to verify that the two parts of (28.65) are equal. With the abbreviation

$$\mathbf{T}(\mathbf{r}_A - \mathbf{r}_B) = \frac{1}{L^3} \sum_{q,s} \frac{1}{q^2} \epsilon_{qs} \epsilon_{qs} e^{i q \cdot (\mathbf{r}_A - \mathbf{r}_B)}, \tag{28.66}$$

the effective Hamiltonian hence is given by

$$\hat{H}_2^{\text{eff}} = -\frac{1}{\epsilon_0 c_0^2} \frac{q_A q_B}{m_A m_B} \hat{\mathbf{p}}_A \cdot \mathbf{T}(\mathbf{r}_A - \mathbf{r}_B) \cdot \hat{\mathbf{p}}_B. \quad (28.67)$$

The Hamiltonian operator in (28.67), which is associated with the one-photon exchange process in a certain limit, represents the first dynamic correction to the Coulomb interaction Hamiltonian, as we now shall realize.

28.3.2 Delay and Magnetic Corrections to the Coulomb Interaction

To gain further insight in the physical structure of $\hat{H}_2^{\text{eff}}$, let us start from the continuum approximation to the tensor in (28.66) that is, with $\mathbf{R} = \mathbf{r}_A - \mathbf{r}_B$,

$$\begin{aligned} \mathbf{T}(\mathbf{R}) &= \sum_s \int_{-\infty}^{\infty} q^{-2} \epsilon_{qs} \epsilon_{qs} e^{i\mathbf{q} \cdot \mathbf{R}} \frac{d^3 q}{(2\pi)^3} \\ &= \int_{-\infty}^{\infty} q^{-2} (U - \hat{\mathbf{q}} \hat{\mathbf{q}}) e^{i\mathbf{q} \cdot \mathbf{R}} \frac{d^3 q}{(2\pi)^3}. \end{aligned} \quad (28.68)$$

The integral in (28.68) can be calculated, and let me now indicate how this is done in a convenient manner by regularization of the integrand. The regularization consists in a replacement of the denominator q^2 by $q^2 + \eta^2$, where by the end of the calculation one assumes that η is an infinitesimally small positive number. It is useful first to consider the integral

$$F(R; \eta) = \int_{-\infty}^{\infty} \frac{e^{i\mathbf{q} \cdot \mathbf{R}}}{q^2 (q^2 + \eta^2)} \frac{d^3 q}{(2\pi)^3}. \quad (28.69)$$

It is a straightforward matter to carry out the integrations in (28.69) in spherical coordinates if one places the polar axis along the direction of $\mathbf{R}$. As the reader may show, the result one obtains is

$$F(R; \eta) = \frac{1}{4\pi R} \frac{1}{\eta^2} (1 - e^{-\eta R}). \quad (28.70)$$

If the Cartesian components of $\mathbf{R}$ and $\mathbf{q}$ are denoted by R_i and q_i ($i = x, y, z$), it appears from (28.69) that

$$\frac{\partial^2 F(R; \eta)}{\partial R_i \partial R_j} = - \int_{-\infty}^{\infty} \frac{q_i q_j e^{i\mathbf{q} \cdot \mathbf{R}}}{q^2 (q^2 + \eta^2)} \frac{d^3 q}{(2\pi)^3}. \quad (28.71)$$

On the basis of (9.62) and (28.71) it follows that the ij th component of the tensor $\mathbf{T}(\mathbf{R})$, i.e.,

$$T_{ij}(\mathbf{r}) = \int_{-\infty}^{\infty} \left(\delta_{ij} - \frac{q_i q_j}{q^2} \right) \frac{e^{i\mathbf{q} \cdot \mathbf{R}}}{q^2} \frac{d^3 q}{(2\pi)^3}, \quad (28.72)$$

is given by

$$T_{ij}(\mathbf{R}) = \frac{\delta_{ij}}{4\pi R} + \lim_{\eta \rightarrow 0^+} \left\{ \frac{\partial^2 F(R; \eta)}{\partial R_i \partial R_j} \right\}. \quad (28.73)$$

If F' and F'' denote the first and second derivatives of F with respect to R one has

$$\frac{\partial^2 F}{\partial R_i \partial R_j} = \delta_{ij} \frac{F'}{R} + \frac{R_i R_j}{R^2} \left(F'' - \frac{F'}{R} \right). \quad (28.74)$$

The right-hand-side of (28.74) is easily calculated from (28.70), and in the limit $\eta \rightarrow 0^+$ one then obtains

$$\lim_{\eta \rightarrow 0^+} \left(\frac{\partial^2 F(R; \eta)}{\partial R_i \partial R_j} \right) = -\frac{\delta_{ij}}{8\pi R} + \frac{R_i R_j}{8\pi R^3}. \quad (28.75)$$

By combining (28.73) and (28.75), one reaches the following result:

$$\mathbf{T}(\mathbf{R}) = \frac{1}{8\pi R} \left(\mathbf{U} + \hat{\mathbf{R}} \hat{\mathbf{R}} \right), \quad (28.76)$$

where as usual $\hat{\mathbf{R}} = \mathbf{R}/R$. In view of (28.76), it appears that the effective Hamiltonian in (28.67) has the form

$$\hat{H}_2^{\text{eff}} = \hat{\Delta}_1 + \hat{\Delta}_2, \quad (28.77)$$

where

$$\hat{\Delta}_1 = -\frac{q_A q_B}{8\pi \epsilon_0 m_A m_B c_0^2} \frac{\hat{\mathbf{p}}_A \cdot \hat{\mathbf{p}}_B}{|\mathbf{r}_A - \mathbf{r}_B|}, \quad (28.78)$$

and

$$\hat{\Delta}_2 = -\frac{\mu_0 q_A q_B}{8\pi m_A m_B} \frac{\hat{\mathbf{p}}_A \cdot (\mathbf{r}_A - \mathbf{r}_B)(\mathbf{r}_A - \mathbf{r}_B) \cdot \hat{\mathbf{p}}_B}{|\mathbf{r}_A - \mathbf{r}_B|^3}. \quad (28.79)$$

It is instructive to look at the two corrections ($\hat{\Delta}_1, \hat{\Delta}_2$) to the Coulomb Hamiltonian from a classical perspective. Let us thus study the energy, H_A , of particle A as it moves in the electromagnetic field created by particle B. In the Coulomb gauge we have

$$H_A = \frac{\mathbf{p}_A^2}{2m_A} + V_{\text{Coul}} - \frac{q_A}{m_A} \mathbf{p}_A \cdot \mathbf{A}_T(\mathbf{r}_A, t), \quad (28.80)$$

and in this gauge the scalar potential is given correctly to all orders as the instantaneous Coulomb potential. For the present purpose it is sufficient to calculate the transverse vector potential acting on particle A, viz.,

$$\mathbf{A}_T(\mathbf{r}_A, t) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \mathbf{J}_T \left(\mathbf{r}', t - \frac{|\mathbf{r}_A - \mathbf{r}'|}{c_0} \right) \frac{d^3 r'}{|\mathbf{r}_A - \mathbf{r}'|}, \quad (28.81)$$

in the nonretarded limit. Thus,

$$\mathbf{A}_T(\mathbf{r}_A, t) = \frac{\mu_0}{4\pi} \int_{-\infty}^{\infty} \mathbf{J}_T(\mathbf{r}', t) \frac{d^3 r'}{|\mathbf{r}_A - \mathbf{r}'|}, \quad (28.82)$$

where $\mathbf{J}_T(\mathbf{r}', t)$ is the transverse current density associated to the motion of particle B. Since the current density of this is given by

$$\mathbf{J}(\mathbf{r}, t) = q_B \mathbf{v}_B(t) \delta(\mathbf{r} - \mathbf{r}_B(t)), \quad (28.83)$$

we obtain

$$\begin{aligned} \mathbf{J}_T(\mathbf{r}', t) &= \int_{-\infty}^{\infty} \delta_T(\mathbf{r}' - \mathbf{r}'') \cdot \mathbf{J}(\mathbf{r}'', t) d^3 r'' \\ &= q_B \mathbf{v}_B(t) \cdot \delta_T(\mathbf{r}' - \mathbf{r}_B(t)), \end{aligned} \quad (28.84)$$

and hence

$$\mathbf{A}_T(\mathbf{r}_A, t) = \frac{\mu_0 q_B}{4\pi} \mathbf{v}_B(t) \cdot \left\{ \int_{-\infty}^{\infty} \delta_T(\mathbf{r}' - \mathbf{r}_B(t)) \frac{d^3 r'}{|\mathbf{r}_A(t) - \mathbf{r}'|} \right\}. \quad (28.85)$$

The integral in the curly bracket can only be a function of the vectorial distance between the particles, and the substitution $\mathbf{r}' = \mathbf{r}_0 + \mathbf{r}_A$ makes this manifest. Thus,

$$\begin{aligned} f(\mathbf{r}_A - \mathbf{r}_B) &\equiv \int_{-\infty}^{\infty} \delta_T(\mathbf{r}' - \mathbf{r}_B(t)) \frac{d^3 r'}{|\mathbf{r}_A(t) - \mathbf{r}'|} \\ &= \int_{-\infty}^{\infty} \delta_T(\mathbf{r}_A - \mathbf{r}_B + \mathbf{r}_0) \frac{d^3 r_0}{r_0}. \end{aligned} \quad (28.86)$$

In the order to carry out the integration in (28.86) one represents the functions δ_T and r_0^{-1} by their Fourier integral transforms. Hence,

$$f(\mathbf{r}_A - \mathbf{r}_B) = \int_{-\infty}^{\infty} \frac{4\pi}{(q')^2} e^{iq' \cdot \mathbf{r}_0} \left(U - \frac{\mathbf{q}\mathbf{q}}{q^2} \right) e^{iq \cdot (\mathbf{r}_A - \mathbf{r}_B + \mathbf{r}_0)} \frac{d^3 q}{(2\pi)^3} \frac{d^3 q'}{(2\pi)^3} d^3 r_0. \quad (28.87)$$

The integration over $\mathbf{r}_0$ brings in the delta function $\delta(\mathbf{q}' + \mathbf{q})$, and this in turn enables us to carry out the integration over the $\mathbf{q}'$ -space, so that

$$f(\mathbf{r}_A - \mathbf{r}_B) = 4\pi \int_{-\infty}^{\infty} \frac{1}{q^2} \left(U - \frac{\mathbf{q}\mathbf{q}}{q^2} \right) e^{iq \cdot (\mathbf{r}_A - \mathbf{r}_B)} \frac{d^3 q}{(2\pi)^3}. \quad (28.88)$$

The integral in (28.88) we have encountered before; it is just the tensor $\mathbf{T}$, given on integral form in (28.68) and explicitly by the expression in (28.76). With

$$f(\mathbf{r}_A - \mathbf{r}_B) = 4\pi \mathbf{T}(\mathbf{r}_A - \mathbf{r}_B), \quad (28.89)$$

it appears that the transverse vector potential, acting on particle A and stemming from particle B, to order $(v/c_0)^2$ is given by

$$\mathbf{A}_T(\mathbf{r}_A, t) = \mu_0 q_B \mathbf{T}(\mathbf{r}_A(t) - \mathbf{r}_B(t)) \cdot \mathbf{v}_B(t). \quad (28.90)$$

By inserting this result into (28.80) it appears that the classical energy of particle A becomes

$$H_A = \frac{\mathbf{p}_A^2}{2m_A} + V_{\text{Coul}} - \mu_0 q_A q_B \mathbf{v}_A \cdot \mathbf{T}(\mathbf{r}_A - \mathbf{r}_B) \cdot \mathbf{v}_B. \quad (28.91)$$

In (28.91), the interaction energy between A and B, given by the last two terms, has been transferred (arbitrarily) to particle A. To obtain the total energy of the two-particle system, one just needs to add the kinetic energy of particle B, $\hat{\mathbf{p}}_B^2/(2m_B)$, to (28.91). The first correction to the Coulomb interaction energy hence is

$$\begin{aligned} -\mu_0 q_A q_B \mathbf{v}_A \cdot \mathbf{T}(\mathbf{r}_A - \mathbf{r}_B) \cdot \mathbf{v}_B &= -\frac{q_A q_B}{8\pi\epsilon_0 m_A m_B c_0^2} \frac{1}{|\mathbf{r}_A - \mathbf{r}_B|} \\ &\times \left[\mathbf{p}_A \cdot \mathbf{p}_B + \frac{\mathbf{p}_A \cdot (\mathbf{r}_A - \mathbf{r}_B)(\mathbf{r}_A - \mathbf{r}_B) \cdot \mathbf{p}_B}{|\mathbf{r}_A - \mathbf{r}_B|^2} \right]. \end{aligned} \quad (28.92)$$

The classical result in (28.92) is in complete correspondence with the quantum operator correction, $\hat{\Delta}_1 + \hat{\Delta}_2$, given via (28.78) and (28.79).

The technique we have used to derive the effective Hamiltonian $\hat{H}_2^{\text{eff}}$ can also be applied to the relativistic electrodynamics of spin-1/2 particles as described by the Dirac equation. In this case the Hamiltonian describing the interaction of the particle (charge q) with the transverse field is given by $-c_0 q \hat{\boldsymbol{\alpha}} \cdot \hat{\mathbf{A}}_T$, where $c_0 \hat{\boldsymbol{\alpha}}$ is the relativistic velocity operator. The effective Hamiltonian describing the correction to the Coulomb energy now takes the form

$$\hat{\Delta}_B = -\frac{q_A q_B}{8\pi\epsilon_0} \frac{1}{|\mathbf{r}_A - \mathbf{r}_B|} \left[\hat{\boldsymbol{\alpha}}_A \cdot \hat{\boldsymbol{\alpha}}_B + \frac{\hat{\boldsymbol{\alpha}}_A \cdot (\mathbf{r}_A - \mathbf{r}_B)(\mathbf{r}_A - \mathbf{r}_B) \cdot \hat{\boldsymbol{\alpha}}_B}{|\mathbf{r}_A - \mathbf{r}_B|^2} \right]. \quad (28.93)$$

The interaction given by (28.93) is known as the Breit interaction [371], and in a certain approximation it describes the transverse-photon mediated coupling between the two particles.

28.3.3 Momentum Exchange

It may be useful here to make a few comments on how the photon momentum exchange appears in the interaction between our charged particles. For this purpose we return to (28.57). The free single-particle states entering the various matrix elements are eigenstates of the momentum operator, and they therefore have the generic form

$$\langle \mathbf{r} | \mathbf{p} \rangle = (2\pi)^{-3/2} \exp\left(\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r}\right) \quad (28.94)$$

in the $\{\mathbf{r}\}$ -representation, when normalized in the Dirac sense, i.e., with an inner product given by

$$\langle \mathbf{p}' | \mathbf{p} \rangle = (2\pi)^{-3} \int_{-\infty}^{\infty} e^{i(\mathbf{p}-\mathbf{p}') \cdot \mathbf{r} / \hbar} d^3 r = \delta(\mathbf{p} - \mathbf{p}'). \quad (28.95)$$

Since

$$\begin{aligned} \langle \mathbf{p}_A'', \mathbf{p}_B'' | \hat{\mathbf{p}}_B e^{-i\mathbf{q} \cdot \mathbf{r}_B} | \mathbf{p}_A, \mathbf{p}_B \rangle &= \langle \mathbf{p}_A'' | \mathbf{p}_A \rangle \langle \mathbf{p}_B'' | e^{-i\mathbf{q} \cdot \mathbf{r}_B} | \mathbf{p}_B \rangle \mathbf{p}_B \\ &= \hbar^3 \mathbf{p}_B \delta(\mathbf{p}_A'' - \mathbf{p}_A) \delta(\mathbf{p}_B'' - \mathbf{p}_B + \hbar \mathbf{q}) \end{aligned} \quad (28.96)$$

it appears that in this transition from the initial state to the intermediate state, particle A is unaffected and particle B emits a photon of momentum $\hbar \mathbf{q}$. The subsequent transition from the intermediate state to the final state involves the matrix element

$$\langle \mathbf{p}_A', \mathbf{p}_B' | \hat{\mathbf{p}}_A e^{i\mathbf{q} \cdot \mathbf{r}_A} | \mathbf{p}_A'', \mathbf{p}_B'' \rangle = \hbar^3 (\mathbf{p}_A' - \hbar \mathbf{q}) \delta(\mathbf{p}_B' - \mathbf{p}_B'') \delta(\mathbf{p}_A'' - \mathbf{p}_A' + \hbar \mathbf{q}), \quad (28.97)$$

and describes a process in which particle B is unaffected and particle A absorbs a photon of momentum $\hbar \mathbf{q}$. The entire process

$$\begin{aligned} \langle \mathbf{p}_A', \mathbf{p}_B' | \hat{\mathbf{p}}_A e^{i\mathbf{q} \cdot \mathbf{r}_A} | \mathbf{p}_A'', \mathbf{p}_B'' \rangle \langle \mathbf{p}_A'', \mathbf{p}_B'' | \hat{\mathbf{p}}_B e^{-i\mathbf{q} \cdot \mathbf{r}_B} | \mathbf{p}_A, \mathbf{p}_B \rangle \\ = \hbar^6 \mathbf{p}_A \mathbf{p}_B \delta(\mathbf{p}_A' - \mathbf{p}_A - \hbar \mathbf{q}) \delta(\mathbf{p}_B' - \mathbf{p}_B + \hbar \mathbf{q}), \end{aligned} \quad (28.98)$$

thus corresponds to an electromagnetic interaction where a transverse photon is emitted by B and reabsorbed by A. Besides this process one has a process, related to the (A $\leftrightarrow$ B)-term in (28.57), describing the emission of a transverse photon from A and reabsorption of this photon by B.

In a process where a nonrelativistic free particle changes its momentum from $\mathbf{p}$ to $\mathbf{p} \pm \hbar \mathbf{q}$, the inequalities in (28.60) are satisfied provided

$$\begin{aligned} \frac{1}{\hbar} \left| \frac{(\mathbf{p} \pm \hbar \mathbf{q})^2}{2m} - \frac{p^2}{2m} \right| &= \frac{1}{m} \left| \mathbf{q} \cdot \left(\frac{\hbar \mathbf{q}}{2} \pm \mathbf{p} \right) \right| \\ &< \frac{q}{m} \left| \mathbf{p} \pm \frac{1}{2} \hbar \mathbf{q} \right| < \omega_q, \end{aligned} \quad (28.99)$$

or equivalently

$$\left| \mathbf{p} \pm \frac{1}{2} \hbar \mathbf{q} \right| < mc_0. \quad (28.100)$$

Qualitatively speaking, the photon momentum transfer must be much smaller than mc_0 , m being the particle rest mass.

28.4 Van der Waals Interaction Between Two Neutral Particles

We now consider the interaction between two neutral particles, e.g., atoms. From a qualitative point of view, the character of the interaction changes significantly with the order of magnitude of the distance R between the particles. Thus, when R is comparable to the extensions of the electronic wave functions of the particles these attract each other and tend to form a single entity. In the case of two hydrogen atoms, for which the relevant atomic dimension is of the order of the Bohr radius, a H_2 molecule is formed and the characteristic R has such a value that the potential energy of the system has a minimum. In the molecular regime the electrons can move between the particles. Electron exchange requires however that the electronic wave functions of the particles overlap in space. Since for each particle the tail of the electronic wave function, roughly speaking, decays exponentially with the distance from the centre of mass, the interaction phenomenon changes completely when R exceeds a few Bohr radii in the atomic case. The interaction between neutral particles close to each other, but not in electronic contact, in a sense has the character of an electrostatic interaction between the electric dipole moments of the particles. The interaction is attractive, and the interaction energy decreases with the distance as R^{-6} . This so-called Van der Waals interaction is of great importance in near-field electrodynamics [24]. At larger distances the interaction energy between the particles decreases more rapidly, viz., as R^{-7} . In physical chemistry the Van der Waals mechanism plays a particularly important role in the interaction between particles which have no valence electrons (rare gas atoms, stable molecules, etc.). In this section, the physics related to the R^{-6} -interaction is in focus.

28.4.1 Interaction from the Power–Zienau–Woolley Point of View

Let us now consider two electrically neutral particles (atoms, molecules, etc.) A and B, with centre of masses located at $\mathbf{r}_A$ and $\mathbf{r}_B$. The charges building up particle A and B are denoted by indices α (or α') and β (or β'), respectively. With the choice made in Sect. 25.2.1, the polarization density of particle A, measured relative to its centre of mass, is given by (cf. (25.20))

$$\mathbf{P}^A(\mathbf{r}) = \sum_{\alpha} \int_0^1 q_{\alpha} \mathbf{\Delta}_{\alpha} \delta(\mathbf{r} - \mathbf{r}_A - u \mathbf{\Delta}_{\alpha}) du, \quad (28.101)$$

where $\mathbf{\Delta}_{\alpha} = \mathbf{r}_{\alpha} - \mathbf{r}_A$ is the position vector of particle α (charge q_{α}) measured relative to $\mathbf{r}_A$. Similarly, the polarization density of particle B measured relative to $\mathbf{r}_B$ will be

$$\mathbf{P}^B(\mathbf{r}) = \sum_{\beta} \int_0^1 q_{\beta} \mathbf{\Delta}_{\beta} \delta(\mathbf{r} - \mathbf{r}_B - u \mathbf{\Delta}_{\beta}) du, \quad (28.102)$$

where $\mathbf{\Delta}_\beta = \mathbf{r}_\beta - \mathbf{r}_B$.

In Sect. 25.5.2 we used a certain unitary transformation (25.95) to transform the quantum description from the Coulomb to the Poincaré gauge. In the presentation given the positions of all the charges were measured from a single point of reference, taken as the origo; see (25.20) and (25.97), and the result we arrived at for the Hamilton operator is given in (25.127)–(25.130). In the case where one has two localized system of charges with different reference points, a unitary operator of the form given in (25.95) can still be used in a transformation from the Coulomb to the extended Poincaré description, but the operator $\hat{F}$ in (25.96) must be replaced by a new one, namely,

$$\hat{F} = - \int_{-\infty}^{\infty} (\hat{\mathbf{P}}^A(\mathbf{r}) + \hat{\mathbf{P}}^B(\mathbf{r})) \cdot \hat{\mathbf{A}}_T(\mathbf{r}) d^3r. \quad (28.103)$$

If the reader has familiarized himself with the calculation in Sects. 25.5.2–25.5.4, it is pretty clear that one ends up with a Hamiltonian operator having the following structure (leaving out superscript P):

$$\hat{H} = \hat{H}_F + \hat{H}_P^A + \hat{H}_P^B + \hat{H}_I^A + \hat{H}_I^B + \hat{H}_I^{AB}. \quad (28.104)$$

The first term on the right side of (28.104), $\hat{H}_F$, is the Hamiltonian of the radiation field, given by either of the equivalent expressions in (25.129). The next two terms, $\hat{H}_P^A$ and $\hat{H}_P^B$, are the particle Hamiltonians of the two systems A and B. The Hamiltonians are given by expressions which are copies of the one in (25.128). Likewise, the two interactions Hamiltonians, $\hat{H}_I^A$ and $\hat{H}_I^B$, are given by expressions of the form in (25.130). These interaction Hamiltonians describe the coupling between the particles of each subsystem and the prevailing radiation field (given in terms of the Poincaré vector potential, $\hat{\mathbf{A}}^P$, and the field momentum, $\hat{\mathbf{\Pi}}$, operators). Since the radiation field is a common quantity for the entire system (A+B), the terms $\hat{H}_I^A$ and $\hat{H}_I^B$ account for a field mediated interaction between the two particle subsystems. The presence of the last term, $\hat{H}_I^{AB}$, in (28.104), which is given by

$$\hat{H}_I^{AB} = \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \hat{\mathbf{P}}_T^A(\mathbf{r}) \cdot \hat{\mathbf{P}}_T^B(\mathbf{r}) d^3r + \sum_{\alpha, \beta} \frac{q_\alpha q_\beta}{4\pi\epsilon_0 |\mathbf{r}_\alpha - \mathbf{r}_\beta|}, \quad (28.105)$$

seems to indicate that there exists a nonradiative interaction between the two particles. In case, this interaction is the sum of the Coulomb interaction energy (last term) and an energy belonging to the overlap of the transverse parts of the two particle polarization densities. As it stands, $\hat{H}_I^{AB}$ will be nonvanishing only if the two neutral particles are in near-field contact. Amazingly, the term $\hat{H}_I^{AB}$ turns out to be identically zero, unless the particles are in electronic contact.

In order to show this the Coulomb interaction energy (operator),

$$\hat{V}_{\text{Coul}}^{\text{AB}} = \frac{1}{4\pi\epsilon_0} \sum_{\alpha,\beta} \frac{q_\alpha q_\beta}{|\mathbf{r}_\alpha - \mathbf{r}_\beta|}, \quad (28.106)$$

is written as a difference between the Coulomb energy of the total system, $\hat{V}_{\text{Coul}}^{\text{A+B}}$, and the sum of the Coulomb energies of the two (isolated) subsystems, $\hat{V}_{\text{Coul}}^{\text{A}}$ and $\hat{V}_{\text{Coul}}^{\text{B}}$,

$$\hat{V}_{\text{Coul}}^{\text{AB}} = \hat{V}_{\text{Coul}}^{\text{A+B}} - \hat{V}_{\text{Coul}}^{\text{A}} - \hat{V}_{\text{Coul}}^{\text{B}}. \quad (28.107)$$

We know from the analysis in subsection 9.3.2 that the Coulomb energy of an assembly of charges (9.68) can be expressed in terms of the longitudinal electric field of these charges (9.59). Utilizing this, one has

$$\begin{aligned} \hat{V}_{\text{Coul}}^{\text{AB}} &= \frac{\epsilon_0}{2} \int_{-\infty}^{\infty} \left[(\hat{\mathbf{E}}_{\text{L}}^{\text{A}}(\mathbf{r}) + \hat{\mathbf{E}}_{\text{L}}^{\text{B}}(\mathbf{r}))^2 - (\hat{\mathbf{E}}_{\text{L}}^{\text{A}}(\mathbf{r}))^2 - (\hat{\mathbf{E}}_{\text{L}}^{\text{B}}(\mathbf{r}))^2 \right] d^3r \\ &= \epsilon_0 \int_{-\infty}^{\infty} \hat{\mathbf{E}}_{\text{L}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{E}}_{\text{L}}^{\text{B}}(\mathbf{r}) d^3r. \end{aligned} \quad (28.108)$$

Since the longitudinal part of the displacement field is zero for a globally neutral system (see Sect. 10.4) one can use the connection

$$\epsilon_0 \hat{\mathbf{E}}_{\text{L}}(\mathbf{r}) = -\hat{\mathbf{P}}_{\text{L}}(\mathbf{r}) \quad (28.109)$$

to express the Coulomb interaction energy in the form

$$\hat{V}_{\text{Coul}}^{\text{AB}} = \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \hat{\mathbf{P}}_{\text{L}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_{\text{L}}^{\text{B}}(\mathbf{r}) d^3r. \quad (28.110)$$

When this formula is used in (28.105), one obtains

$$\begin{aligned} \hat{H}_{\text{I}}^{\text{AB}} &= \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \left(\hat{\mathbf{P}}_{\text{T}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_{\text{T}}^{\text{B}}(\mathbf{r}) + \hat{\mathbf{P}}_{\text{L}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_{\text{L}}^{\text{B}}(\mathbf{r}) \right) d^3r \\ &= \frac{1}{\epsilon_0} \int_{-\infty}^{\infty} \mathbf{P}^{\text{A}}(\mathbf{r}) \cdot \mathbf{P}^{\text{B}}(\mathbf{r}) d^3r. \end{aligned} \quad (28.111)$$

The last member of (28.111) follows from the fact that

$$\int_{-\infty}^{\infty} \hat{\mathbf{P}}_{\text{T}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_{\text{L}}^{\text{B}}(\mathbf{r}) d^3r = \int_{-\infty}^{\infty} \hat{\mathbf{P}}_{\text{L}}^{\text{A}}(\mathbf{r}) \cdot \hat{\mathbf{P}}_{\text{T}}^{\text{B}}(\mathbf{r}) d^3r = 0. \quad (28.112)$$

The result in (28.111) shows that there is no instantaneous interaction between A and B, unless the polarization fields themselves overlap. The near-field interaction

between the particles thus is ascribed exclusively to the exchange of transverse photons in the Power–Zienau–Woolley picture.

28.4.2 Exchange of Virtual Transverse Photons

Let us assume that the charge distribution in each of the two particles is so strongly localized that one can use the electric dipole approximation. From the analysis in Sect. 27.3 it then follows that the interaction Hamiltonian in (28.104) is given by

$$\hat{H}_I^A + \hat{H}_I^B = -\epsilon_0^{-1} \hat{\mathbf{d}}^A \cdot \hat{\mathbf{D}}(\mathbf{r}_A) - \epsilon_0^{-1} \hat{\mathbf{d}}^B \cdot \hat{\mathbf{D}}(\mathbf{r}_B), \quad (28.113)$$

where

$$\hat{\mathbf{d}}^A = \sum_{\alpha} q_{\alpha} \mathbf{A}_{\alpha}, \quad (28.114)$$

and

$$\hat{\mathbf{d}}^B = \sum_{\beta} q_{\beta} \mathbf{A}_{\beta} \quad (28.115)$$

are the electric dipole moment operators of the particles A and B in the $\{\mathbf{r}\}$ -representation. As indicated, the ED-moments are measured relative to the two centre of masses (For a neutral particle the ED-moment is of course independent of the chosen point of reference). On the basis of the interaction Hamiltonian in (28.113) one is able to study the Van der Waals interaction in great detail, among other aspects for instance the energy transfer between the particles and the role of causality. Here, we shall just discuss how the energy of the two particles in their ground state (which is assumed to have no permanent ED-moment) is modified by the photon exchange process in the limit where the energy of the virtual photons is high, but first a few general remarks are given.

Let the ground state of the two particles be $|a\rangle$ and $|b\rangle$, and let us assume that they are placed in a photon vacuum, $|0\rangle$. Initially, the global particle–field system hence is in the quantum state

$$|\psi_i\rangle = |a, b; 0\rangle = |a, b\rangle \otimes |0\rangle = |a\rangle \otimes |b\rangle \otimes |0\rangle. \quad (28.116)$$

In order to investigate in a perturbative approach how the ground state of the system is modified by the exchange of transverse photons various types of matrix elements involving the interaction Hamiltonian must be calculated. In all cases the initial and final states of the global system must be identical. This implies that at least two photons have to be exchanged between the particles. In general, the exchange process always involves *pairs* of photons. The necessity for pair-exchange may be illustrated as follows: The emission of a photon by particle A is accompanied by a transition of this particle from the ground state $|a\rangle$ to an excited state $|a'\rangle$. If A is to return to the ground state a subsequent photon absorption is required. In lowest order, the

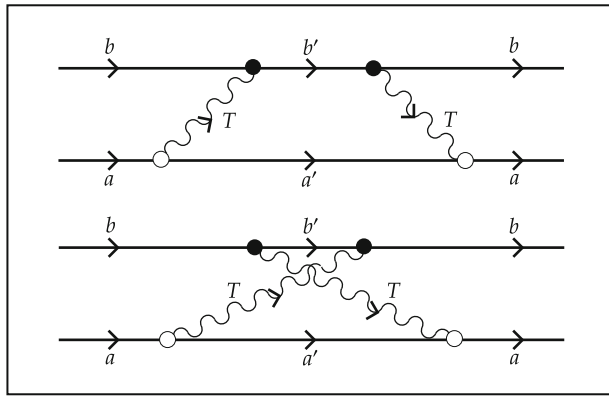


Fig. 28.2 Feynman diagrams describing the (main part of the) Van der Waals interaction between two (a, b) neutral atoms in the ground states $|a\rangle$ and $|b\rangle$. Exchange of *two* transverse photons (T) allows a return of the particles to their ground states after having been in the intermediate states $|a'\rangle$ and $|b'\rangle$. Vertices in which atom a is involved are denoted by the symbol *bullet*, and those involving b bear the symbol *circle*

process $|a\rangle \rightarrow |a'\rangle \rightarrow |a\rangle$ thus requires two photons, but so far particle B has not been involved. The interaction between A and B can be activated if the photon emitted by A is absorbed by B, which goes into an excited state, say $|b'\rangle$. After this particular one-photon exchange the state of the global system is $|a', b'; 0\rangle$. To return from here to the original state in (28.116), a photon must be emitted by B and then reabsorbed by A. Altogether, an interaction of the type described above requires an exchange of one pair of photons. Two examples of Feynman diagrams for the process are shown in Fig. 28.2. Since the temporal order of the four elementary processes may be interchanged, ten other Feynman diagrams are needed to describe the lowering of the ground-state energy in a Van der Waals interaction of lowest order. These diagrams are shown in Fig. 28.3. The one-photon exchange process, which brings the global field-particle system from the initial state $|a, b; 0\rangle$ to the excited state $|a', b'; 0\rangle$, can be calculated by a procedure analogous to the one we used to obtain the $\mathbf{p} \cdot \mathbf{A}_T$ -interaction contribution to the single-photon exchange between two charged particles in Sect. 28.3.1. In the matrix elements of (28.53) we just need to make the replacements

$$\frac{q_I}{m_I} \hat{\mathbf{p}}_I \cdot \hat{\mathbf{A}}_T(\mathbf{r}_I) \Rightarrow \frac{1}{\epsilon_0} \hat{\mathbf{d}}_I \cdot \hat{\mathbf{D}}(\mathbf{r}_I), \quad I = A, B. \quad (28.117)$$

By means of the expression given (25.126) for $\hat{\mathbf{H}}(\mathbf{r}) = -\hat{\mathbf{D}}_T(\mathbf{r}) = -\hat{\mathbf{D}}(\mathbf{r})$ one obtains

$$\langle 0 | \hat{\mathbf{D}}(\mathbf{r}_A) | \mathbf{q}s \rangle \langle \mathbf{q}s | \hat{\mathbf{D}}(\mathbf{r}_B) | 0 \rangle = \frac{1}{L^3} \frac{\epsilon_0 \hbar \omega_q}{2} \epsilon_{qs} \epsilon_{qs} e^{i\mathbf{q} \cdot (\mathbf{r}_A - \mathbf{r}_B)}. \quad (28.118)$$

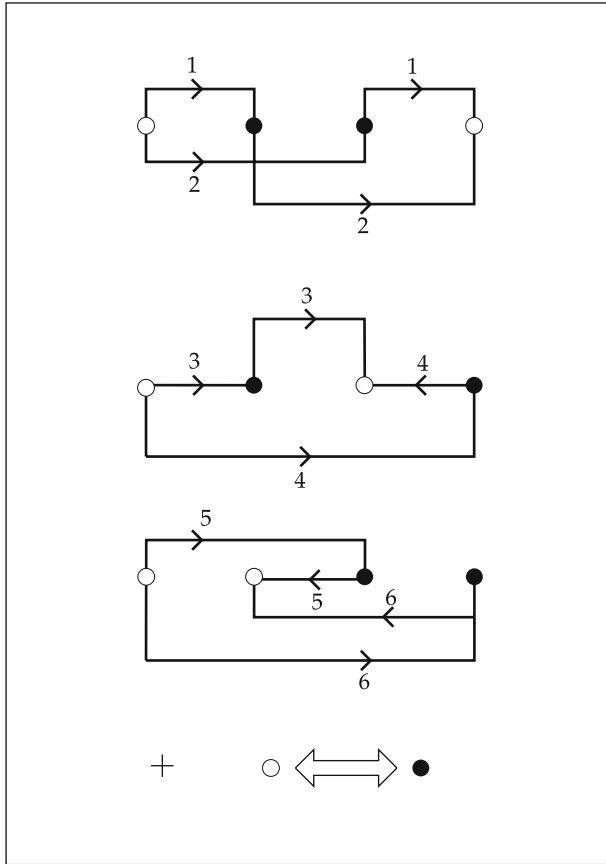


Fig. 28.3 Besides the two Feynman diagrams in Fig. 28.2, ten other diagrams are needed to describe the Van der Waals interaction between the two neutral atoms to lowest order. These are obtained by exchanging the temporal order of the four vertices. All the twelve diagrams are shown in this figure. As in the previous figure, the symbols *bullet* and *circle* refer to atom *a* and *b*, respectively, and the time runs from left to right. Six sequences are shown in detail, and numbered 1–6, and the remaining six are obtained by the exchange $\bullet \leftrightarrow \circ$. Two sequences are displayed in each of the three diagrams shown

When one carries out the summation over the field modes, it is qualitatively so that field modes with wave numbers $q \geq |\mathbf{r}_A - \mathbf{r}_B|^{-1}$ contribute little: the phase factor $\exp[i\mathbf{q} \cdot (\mathbf{r}_A - \mathbf{r}_B)]$ varies rapidly with q , and these high frequency modes therefore interfere destructively. The low-frequency modes, on the other hand, also contribute little to the sum over modes because their density is low. Altogether, one thus may conclude that the most significant contribution to the one-photon exchange process above comes from photons for which the wavelength is of the order of the distance $|\mathbf{r}_A - \mathbf{r}_B|$ between the particles. Such photons have an energy $\approx \hbar c/|\mathbf{r}_A - \mathbf{r}_B|$. If this energy is much larger than the typical excitation energies of the particles

($|E_{a'} - E_a|, |E_{b'} - E_b|$) approximations analogous to those in the inequalities in (28.60) can be used. Hence, if the distance between the two particles is so small that it satisfies

$$|\mathbf{r}_A - \mathbf{r}_B| \ll c_0 \omega_{aa'}^{-1}, \quad c_0 \omega_{bb'}^{-1}, \quad (28.119)$$

where $\omega_{aa'}$ and $\omega_{bb'}$ are typical Bohr frequencies, the matrix element of relevance for the one-photon exchange process between the two neutral particles, namely

$$\langle a', b'; 0 | \hat{H}_2' | a, b; 0 \rangle_{\text{EXCHANGE}} = \langle a', b' | \hat{H}_2^{\text{eff}} | a, b \rangle, \quad (28.120)$$

is a sandwich containing the effective Hamiltonian

$$\begin{aligned} \hat{H}_2^{\text{eff}} &= -\frac{1}{2\epsilon_0 L^3} \sum_{q,s} \boldsymbol{\epsilon}_{qs} \cdot \hat{\mathbf{d}}^A \hat{\mathbf{d}}^B \cdot \boldsymbol{\epsilon}_{qs} e^{i\mathbf{q} \cdot (\mathbf{r}_A - \mathbf{r}_B)} + (A \leftrightarrow B) \\ &= -\frac{1}{\epsilon_0} \hat{\mathbf{d}}^A \cdot \left[\frac{1}{L^3} \sum_{q,s} \boldsymbol{\epsilon}_{qs} \boldsymbol{\epsilon}_{qs} e^{i\mathbf{q} \cdot (\mathbf{r}_A - \mathbf{r}_B)} \right] \cdot \hat{\mathbf{d}}^B. \end{aligned} \quad (28.121)$$

The last member of (28.121) follows readily upon a substitution $\mathbf{q} \rightarrow -\mathbf{q}$ in the $(A \leftrightarrow B)$ -term. In the continuum limit ($L \rightarrow \infty$), the quantity inside the bracket is just the transverse delta function. The effective Hamiltonian

$$\hat{H}_2^{\text{eff}} = -\frac{1}{\epsilon_0} \hat{\mathbf{d}}^A \cdot \boldsymbol{\delta}_T(\mathbf{r}_A - \mathbf{r}_B) \cdot \hat{\mathbf{d}}^B \quad (28.122)$$

therefore relates to an instantaneous dipole–dipole interaction between the two neutral atoms. For such an interaction, the classical interaction energy W^{AB} is given by the well known expression

$$W^{\text{AB}} = \frac{\mathbf{d}^A \cdot \mathbf{d}^B - 3(\hat{\mathbf{n}} \cdot \mathbf{d}^A)(\hat{\mathbf{n}} \cdot \mathbf{d}^B)}{4\pi\epsilon_0 |\mathbf{r}_A - \mathbf{r}_B|^3}, \quad (28.123)$$

where $\hat{\mathbf{n}}$ is a unit vector in the direction $\mathbf{r}_A - \mathbf{r}_B$.

The effective Hamiltonian in (28.122) has so far been used to couple the ground state $|a, b\rangle$ to the excited state $|a', b'\rangle$. A second one-photon exchange process allows one to deexcite the system from this state back to the ground state. To second order in the effective Hamiltonian, $\hat{H}_2^{\text{eff}}$, the Van der Waals interaction leads to an energy shift, ΔE , of the state $|a, b\rangle$ given by

$$\Delta E = \sum_{\substack{a', b' \\ (\neq a, b)}} \frac{\langle a, b | \hat{H}_2^{\text{eff}} | a', b' \rangle \langle a', b' | \hat{H}_2^{\text{eff}} | a, b \rangle}{E_a + E_b - E_{a'} - E_{b'}}. \quad (28.124)$$

The result in (28.124) follows from standard second-order stationary perturbation theory, assuming that the states are nondegenerate. Since both particles were assumed to be in the initial state $|a, b\rangle = |a\rangle \otimes |b\rangle$, the denominator in (28.124) will be negative. This means that the energy shift ΔE is negative, and the Van der Waals interaction hence lowers the ground-state energy of the system. The expression for $\hat{H}_2^{\text{eff}}$ given in (28.122) varies with the distance between the particles, as $|\mathbf{r}_A - \mathbf{r}_B|^{-3}$, and the Van der Waals interaction energy therefore has the form

$$\Delta E = -\frac{C_6}{|\mathbf{r}_A - \mathbf{r}_B|^6} \quad (28.125)$$

at short distances, where the energy of the most important virtual transverse photons is high. The constant C_6 is positive. From (28.125) one can conclude that the Van der Waals force between A and B is attractive and varies as $|\mathbf{r}_A - \mathbf{r}_B|^{-7}$ when the distance between the particles is sufficiently small.

On the basis of (28.122) and (28.124) it is not difficult to calculate the Van der Waals interaction energy between two hydrogen atoms in the $1s$ ground state (leaving out spin dynamics this state is nondegenerate). I leave this as an exercise for the reader, with the remark that an estimate of the order of magnitude of C_6 can be obtained approximating all the denominators in (28.124) by $E_A + E_B = -2E_1$, $E_1 = me^4/(2\hbar^2) \approx 13.6 \text{ eV}$ being the Rydberg (ionization) energy of the hydrogen atom. It should be noted that the Van der Waals interaction energy between two hydrogen atoms of which one is in the $1s$ ground state and the other in the $2p$ state varies with distance as $|\mathbf{r}_A - \mathbf{r}_B|^{-3}$ and not as $|\mathbf{r}_A - \mathbf{r}_B|^{-6}$. The reason for this originates in the fact that the effective Hamiltonian in (28.122) in this case modifies the energy of the system in first order. The sign of the interaction energy is opposite for the two eigenstates

$$|\psi_{\pm}\rangle = \frac{1}{\sqrt{2}} (|1s, 2p\rangle \pm |2p, 1s\rangle) \quad (28.126)$$

of the two-atom system; it is positive for $|\psi_+\rangle$.

28.5 Casimir Effect: Particle–Surface Interaction

In near-field electrodynamics the interaction between a mesoscopic (or atomic) particle and a (planar) surface of a solid medium is of great interest for various reasons [24, 372]. Thus, the free-space spontaneous emission of an atom will be modified in the presence of a nearby surface, and if the atom is placed between two surfaces important electrodynamic cavity phenomena may occur. In the presence of an electromagnetic surface wave, charged and neutral particles traveling near the surface can be bend in the evanescent tail of the surface wave. The surface-induced modification of the spectral properties of a mesoscopic particle may also be used

to study certain surface properties of solids, e.g., the interaction between surface atoms. If a charged particle moves along a surface with a speed exceeding one of the characteristic phase velocities of the electromagnetic surface modes, it has been predicted that electromagnetic surface shock waves may be generated [5, 162]. These waves which have been named Cherenkov–Landau surface shock waves are physically related to (1) the well known Cherenkov shock waves which can be emitted when a charged particle propagates inside a medium with a speed exceeding the phase velocity of the transverse (bulk polariton) modes of the medium [373, 374] and (2) the Landau shock waves generated when the particle speed is larger than the phase velocity of the longitudinal (bulk plasmon) modes [375]. When a mesoscopic particle is placed near a nonlinear medium, phase conjugation of the outgoing (electric-dipole) radiation from the particle can be used to make so-called quantum dots of light.

A detailed understanding of the electrodynamic particle–surface interaction in general requires a good knowledge of the microscopic electrodynamic (quantum physical) properties of the surface. Green function methods, which take into account that an electromagnetic field emitted from the particle is reflected and transmitted at the surface, are particularly suitable for tackling the microscopic problems [24, 77, 78]. These methods also allow one to take into account field retardation effects, which always are of importance when the particle is outside the rim zone of the surface.

In the present section we shall not study any of the above-mentioned phenomena, but just demonstrate how the Van der Waals interaction can lead to particle–surface attraction. For simplicity, it is assumed that the medium is a perfect conductor (metal, superconductor). Basically, such an assumption is tantamount to a complete electromagnetic decoupling of the conductor from our mesoscopic particle. The only role of the conductor is “to ensure” that the electromagnetic field vanishes completely inside and at the surface at all times. It is further assumed that the particle, which here is treated as an electric dipole, is so close to the surface that field retardation effects can be neglected. Under the afore-mentioned assumptions, the particle–surface coupling mathematically can be treated as an interaction between the dipole and its electrical image on the other side of the surface.

Let the centre of mass of the particle be placed at a distance R from the surface, and let its position vector in Cartesian coordinates be $\mathbf{R} = (0, 0, R)$. The centre of mass of the image of the particle (characterized by the superscript I) thus is located at $\mathbf{R}^I = (0, 0, -R)$. As in Sect. 28.4.2 we assume that our particle is composed of a set of point charges $\{q_\alpha\}$ which positions relative to $\mathbf{R}$ are $\{\Delta_\alpha\}$. With

$$\Delta_\alpha = (\Delta_{\parallel,\alpha}, \Delta_{\perp,\alpha}), \quad (28.127)$$

where $\Delta_{\parallel,\alpha}$ is the vectorial component of the position vector parallel to the surface, and $\Delta_{\perp,\alpha}$ its z -component, the corresponding image point particle is located at

$$\Delta_\alpha^I = (\Delta_{\parallel,\alpha}, -\Delta_{\perp,\alpha}), \quad (28.128)$$

and has a charge $-q_\alpha$. Now, it follows that to the electric dipole moment of the mesoscopic (or atomic) particle, viz.,

$$\mathbf{d} = \sum_{\alpha} q_{\alpha} (\mathbf{\Delta}_{\parallel, \alpha}, \mathbf{\Delta}_{\perp, \alpha}) \equiv (\mathbf{d}_{\parallel}, \mathbf{d}_{\perp}), \quad (28.129)$$

there is associated an image dipole moment

$$\mathbf{d}^I = \sum_{\alpha} (-q_{\alpha}) (\mathbf{\Delta}_{\parallel, \alpha}, -\mathbf{\Delta}_{\perp, \alpha}) = (-\mathbf{d}_{\parallel}, \mathbf{d}_{\perp}). \quad (28.130)$$

Since the particle is so close to the surface that the field retardation is unimportant, we know that the energies of the virtual transverse photons mediating the particle-surface interaction are so high that the effective-Hamiltonian description is valid. From (28.122) we can then deduce that the quantum physical interaction between the particle and its image can be described on the basis of the effective Hamiltonian

$$\hat{H}_2^{\text{eff}} = -\frac{1}{2\epsilon_0} \hat{\mathbf{d}} \cdot \delta_T(2R\hat{z}) \cdot \hat{\mathbf{d}}^I, \quad (28.131)$$

where $\hat{z}$ is a unit vector in the z -direction. The reader will notice that there is an “extra” factor of 2 in the denominator of (28.131). This factor is necessary since the dipole image is fictitious and the field, and thus the field energy, is zero in our ideal conductor. By means of (28.129) and (28.130), and the explicit expression for the transverse delta function given in (9.19), one obtains

$$\hat{H}_2^{\text{eff}} = -\frac{1}{4\pi\epsilon_0} \frac{1}{2} \frac{1}{(2R)^3} (\hat{\mathbf{d}}_{\parallel}^2 + 2\hat{\mathbf{d}}_{\perp}^2). \quad (28.132)$$

Since the conductor is a passive medium here, the only dynamical degrees of freedom are those of the particle. Thus, the fictitious motion of the image dipole is perfectly correlated with the motion of the particle itself, of course. For a particle in the ground state $|a\rangle$, the first-order correction to the ground-state energy, i.e.,

$$\Delta E = \langle a | \hat{H}_2^{\text{eff}} | a \rangle = -\frac{1}{8\pi\epsilon_0} \frac{1}{(2R)^3} \langle a | \hat{\mathbf{d}}_{\parallel}^2 + 2\hat{\mathbf{d}}_{\perp}^2 | a \rangle, \quad (28.133)$$

will in general be different from zero, even for a particle with a spherical charge density distribution. It is seen from (28.133) that the particle is attracted by the surface: The interaction energy is negative and varies with R^{-3} , and the force of attraction therefore varies as R^{-4} . The particle-surface attraction described above is, as mentioned earlier, called the Casimir effect [71, 339].

The Casimir attraction force between two particles which ground states are spherical symmetric, e.g., two hydrogen atoms, will vary as $|\mathbf{r}_A - \mathbf{r}_B|^{-7}$ because there is no first-order correction to the ground-state energy. The reason for this stems

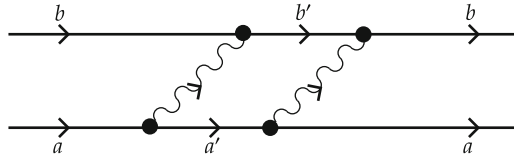


Fig. 28.4 Examples of two-photon processes related to the Casimir–Polder effect (Van der Waals interaction at large inter-particle distance). Two photons are emitted by atom a in the cycle $|a\rangle \rightarrow |a'\rangle \rightarrow |a\rangle$, and after a propagation time which is long compared to the duration of the virtual excitation of the atoms, absorbed in atom b in a cycle $|b\rangle \rightarrow |b'\rangle \rightarrow |b\rangle$

from the fact that the effective interaction Hamiltonian is linear in $\hat{\mathbf{d}}^A$ and $\hat{\mathbf{d}}^B$; see (28.122).

28.6 Remarks on the Casimir–Polder Effect

It appears from the analysis in Sect. 28.4 that a quantum electrodynamic calculation of the Van der Waals interaction requires fourth-order perturbation theory. When the distance between the particles is much less than the typical Bohr wavelength (divided by 2π), i.e.,

$$|\mathbf{r}_A - \mathbf{r}_B| \ll \tilde{\lambda}_{\text{Bohr}}, \quad (28.134)$$

the energy of the virtual transverse photons is high, and the interaction can be described on the basis of the processes shown in Figs. 28.2 and 28.3. At small distances the interaction energy is proportional to $|\mathbf{r}_A - \mathbf{r}_B|^{-6}$.

When the inter-particle distance is so large that

$$|\mathbf{r}_A - \mathbf{r}_B| \gg \tilde{\lambda}_{\text{Bohr}}, \quad (28.135)$$

the energy of the exchanged photons is small compared to the particle excitation energies, and the photon propagation time between the particles thus is long in comparison to the excitation–deexcitation cycles of the particles ($a \rightarrow a' \rightarrow a$, $b \rightarrow b' \rightarrow b$). The overall Van der Waals process now may be considered as a quasi-static two-photon emission process by one of the particles followed by a corresponding quasi-static absorption of this pair of photons by the other particle. An example of a two-photon exchange is shown in the diagram of Fig. 28.4. To determine the distance dependence of the Van der Waals interaction it is important to keep track of the energy defects of the various intermediate states. When the inequality in (28.134) is satisfied, defects $\hbar\omega = \hbar c_0 q$, $E_a + E_b - E_{a'} - E_{b'}$, and $\hbar\omega' = \hbar c_0 q'$ occur, and the appearance of the photon energy twice in the relevant denominator results in the $|\mathbf{r}_A - \mathbf{r}_B|^{-6}$ -dependence of the interaction energy at small distances. When the inequality in (28.135) holds, an energy defect involving the photons only appear in relation to the photon propagation between the particles. The defect, $\hbar\omega + \hbar\omega'$, only shows up once in the relevant denominator, and in the calculation of the Fourier

integrals over the $\mathbf{q}$ and $\mathbf{q}'$ -spaces an extra $|\mathbf{q}|$ (or $|\mathbf{q}'|$)-factor enters. In consequence an additional $|\mathbf{r}_A - \mathbf{r}_B|^{-1}$ -factor appears in the final result. At large distances the Van der Waals interaction energy thus varies as $|\mathbf{r}_A - \mathbf{r}_B|^{-7}$. This more rapid decrease at large distances is called the Casimir–Polder effect [72], as said before.

Chapter 29

Photons in a Manifestly Lorentz-Covariant Theory

Theoretical studies in near-field quantum electrodynamics are seldom carried out in the framework of the so-called covariant formulation, which is so important in relativistic quantum electrodynamics. In a sense this is very natural because near-field investigations up to this date have dealt exclusively with nonrelativistic problems. With this in mind it is understandable that the Coulomb gauge, and gauges related to this by a unitary transformation, have been in focus in classical and quantum near-field electrodynamics. We have seen in previous chapters of this book, however, that the longitudinal and scalar photons play an important conceptual role in the quantum mechanical (first-quantized) photon picture of near-field interactions. The purpose of this chapter is to give readers whose (main) background is in nonrelativistic (near-field) electrodynamics a brief introduction to the covariant formulation of classical and quantum electrodynamics in the free-field limit. Throughout the chapter near-field aspects will be emphasized when adequate.

We begin our description in the classical domain by setting up the free Maxwell equations in a manifestly covariant form, and thereafter we present the Lagrange equations for the free electromagnetic field as they appear in the standard approach. Unfortunately, the standard Lagrangian field density relative to the four-potential is not suitable for carrying out the canonical field quantization because the scalar potential has no conjugate momentum. We therefore switch to a modified Lagrangian density, which is suitable for quantization but only equivalent to the standard Lagrangian density in the Lorenz gauge. The plane-wave expansion of the four-potential is studied, and we discuss how the bridge can be made between the covariant potential description and the gauge and near-field photon concepts introduced earlier in the framework of photon wave mechanics. We end the classical analysis by showing that the free-field Hamiltonian can be written as a superposition of harmonic oscillator terms. The energies belonging to the two transverse and the longitudinal field modes appear in the expected form, but the energies of the scalar modes all show-up with a negative sign in front. This sign is not a problem for the classical theory because the net effect of the longitudinal and scalar modes vanishes in free space.

The covariant formalism is extended to the quantum level by the usual replacement of normal variables by operators. In the quantum domain the classical Lorenz condition is replaced by what I call the Gupta–Bleuler–Lorenz condition, which is

a subsidiary condition on the state vectors in the subspace of the longitudinal and scalar photons. The negative sign mentioned above leads to the problem of negative norms for certain scalar photon states, and to a cross-coupling between the gauge and near-field photon annihilation and creation operators. To overcome this problem we introduce a covariant quantization scheme with an indefinite metric. With a proper choice of metric, the Hamilton operator representing the gauge and near-field degrees of freedom takes the form of a usual superposition of free oscillator energy operators.

We go on with a study of covariant and equal-time commutator relations involving the four-potential and its conjugate momentum, and we finish the chapter with an introduction of the important covariant Feynman photon propagator.

29.1 Covariant Formulation of Classical Free-Field Dynamics

29.1.1 Covariant Notation

It may be useful to begin with a brief summary of the relativistic notation to be used throughout this chapter. Following the usual convention, the components of four-vectors will be labeled by Greek indices, and the components of spatial three-vectors by Latin indices. Contravariant components are indicated with superscript index, and covariant components appear with subscript index. Contra- and covariant vectors (and tensors) per definition are related by means of the (diagonal) metric tensor $g_{\mu\nu}$, with components

$$\left. \begin{aligned} g_{00} &= -g_{11} = -g_{22} = -g_{33} = +1 \\ g_{\mu\nu} &= 0, \text{ if } \mu \neq \nu \end{aligned} \right\}. \quad (29.1)$$

The contravariant space–time four-vector

$$x \equiv \{x^\mu\} = (x^0, x^1, x^2, x^3) = (c_0t, \mathbf{r}) \quad (29.2)$$

thus has an associated covariant vector, $\{x_\mu\}$, with components given by

$$x_\mu = g_{\mu\nu}x^\nu \quad (29.3)$$

with the summation convention: Repeated indices (one contravariant and one covariant) are summed. From (29.1) and (29.3) one has

$$\{x_\mu\} = (x_0, x_1, x_2, x_3) = (x^0, -x^1, -x^2, -x^3) = (c_0t, -\mathbf{r}). \quad (29.4)$$

For what follows the four-component potential (a four-vector only in covariant gauges, e.g., Lorenz gauges)

$$\left. \begin{aligned} \{A^\mu\} &= (A^0, \mathbf{A}) = (c_0^{-1}\phi, \mathbf{A}) \\ \{A_\mu\} &= (A^0, -\mathbf{A}) \end{aligned} \right\}, \quad (29.5)$$

and the current density four-vector

$$\left. \begin{aligned} \{j^\mu\} &= (j^0, \mathbf{j}) = (c_0\rho, \mathbf{j}) \\ \{j_\mu\} &= (j^0, -\mathbf{j}) \end{aligned} \right\}, \quad (29.6)$$

are of particular importance. It is also to be noted that the four-dimensional generalization of the gradient operator transforms like a four-vector:

$$\left. \begin{aligned} \{\partial_\mu\} &\equiv \left\{ \frac{\partial}{\partial x^\mu} \right\} = \left(\frac{1}{c_0} \frac{\partial}{\partial t}, \nabla \right) \\ \{\partial^\mu\} &\equiv \left\{ \frac{\partial}{\partial x_\mu} \right\} = \left(\frac{1}{c_0} \frac{\partial}{\partial t}, -\nabla \right) \end{aligned} \right\}. \quad (29.7)$$

The contravariant metric tensor is defined by $g^{\mu\nu} = g_{\mu\nu}$.

29.1.2 The Free Maxwell Equations in Covariant Form

Starting from the electromagnetic field equations written in terms of the potentials ((2.8) and (2.9)) it readily appears that the components of the four-vector potential satisfy the coupled differential equations

$$\square A^0 + \frac{1}{c_0} \frac{\partial}{\partial t} \left(\nabla \cdot \mathbf{A} + \frac{1}{c_0} \frac{\partial A^0}{\partial t} \right) = 0, \quad (29.8)$$

$$\square \mathbf{A} - \nabla \left(\nabla \cdot \mathbf{A} + \frac{1}{c_0} \frac{\partial A^0}{\partial t} \right) = 0, \quad (29.9)$$

in free space. Since

$$-\square = \partial_\mu \partial^\mu, \quad (29.10)$$

and

$$\nabla \cdot \mathbf{A} + \frac{1}{c_0} \frac{\partial A^0}{\partial t} = \partial_\mu A^\mu, \quad (29.11)$$

the classical field equations in (29.8) and (29.9) can be written in the *apparently* covariant form

$$(\partial_\nu \partial^\nu) A^\mu - \partial^\mu (\partial_\nu A^\nu) = 0, \quad (29.12)$$

for $\mu = 0, 1, 2, 3$. If the quantity $\partial_\mu A^\mu$ (in (29.11)) equals a constant (zero in the Lorenz gauge(s)), $\{A^\mu\}$ is a four-vector, and (29.12) thus has a genuine covariant form.

29.1.3 Lagrange Equations for the Free Field: Standard Approach

It is possible to derive the field equations in (29.12) from a suitable Lagrangian density, as we will see now [155, 178]. We first introduce the covariant antisymmetric field tensor, $F_{\mu\nu}$, by the definition

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \quad (29.13)$$

The contravariant version of the field tensor, given by the transformation

$$F^{\mu\nu} = g^{\mu\omega} g^{\nu\tau} F_{\omega\tau}, \quad (29.14)$$

relates to the four-component potential as follows:

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu. \quad (29.15)$$

Using (2.5) and (2.7), the reader may show that the field tensor also can be expressed in terms of the components of the electric and magnetic field alone. Thus, in matrix form

$$\{F_{\mu\nu}\} = \frac{1}{c_0} \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & -c_0 B_z & c_0 B_y \\ -E_y & c_0 B_z & 0 & -c_0 B_x \\ -E_z & -c_0 B_y & c_0 B_x & 0 \end{pmatrix}. \quad (29.16)$$

The contravariant field tensor may be obtained from (29.16) making the replacement $\mathbf{E} \rightarrow -\mathbf{E}$:

$$\{F^{\mu\nu}(\mathbf{E}, \mathbf{B})\} = \{F_{\mu\nu}(-\mathbf{E}, \mathbf{B})\}. \quad (29.17)$$

The standard Lagrangian density of the electromagnetic field, viz.,

$$\mathcal{L}_F^{\text{ST}} = \frac{\epsilon_0}{2} (\mathbf{E}^2 - \mathbf{B}^2), \quad (29.18)$$

(see (25.35) and (25.37)) can be expressed in terms of the field tensor as follows:

$$\mathcal{L}_F^{\text{ST}} = -\frac{\epsilon_0 c_0^2}{4} F_{\mu\nu} F^{\mu\nu}, \quad (29.19)$$

(with summation over μ and ν). The correctness of this formula is obvious in the view of the relation in (29.17), and the invariance of $\mathcal{L}_F^{\text{ST}}$ under Lorentz transformations is manifest from the form given in (29.19). As mentioned in Sect. 25.3.1 it is possible to derive the Maxwell–Lorentz equations from suitable Lagrange equations relative to the scalar and vector potentials. In the free-field limit the Lagrange equations ($\mu = 0, 1, 2, 3$)

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial \dot{A}_\mu} \right) + \sum_{j=1}^3 \partial_j \left(\frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial (\partial_j A_\mu)} \right) - \frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial A_\mu} = 0 \quad (29.20)$$

therefore must lead to the field equations in (29.12). The Lagrange equations *relative to the potentials* may also be written in the covariant form

$$\sum_{\nu=0}^3 \partial_\nu \left(\frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial (\partial_\nu A_\mu)} \right) - \frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial A_\mu} = 0. \quad (29.21)$$

Unfortunately, the standard Lagrangian density is not suitable for carrying out the field quantization if one wants to treat the scalar and vector potential in a symmetrical manner. In order to understand this let us calculate the conjugate field momenta

$$\Pi_\mu^{\text{ST}} \equiv \frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial \dot{A}_\mu}. \quad (29.22)$$

Since only terms in $\mathcal{L}_F^{\text{ST}}$ which contains the time derivative of A_μ can contribute to Π_μ^{ST} , one gets

$$\begin{aligned} \frac{\partial \mathcal{L}_F^{\text{ST}}}{\partial \dot{A}^\mu} &= -\frac{\epsilon_0 c_0^2}{4} \frac{\partial}{\partial \dot{A}^\mu} (F_{0\mu} F^{0\mu} + F_{\mu 0} F^{\mu 0}) \\ &= \frac{\epsilon_0 c_0^2}{2} \frac{\partial}{\partial \dot{A}^\mu} (F^{0\mu})^2. \end{aligned} \quad (29.23)$$

The last member of (29.23) follows from (29.17) and the antisymmetry of the field tensor. The standard Lagrangian density thus leads to the conjugate field momenta

$$\Pi_\mu^{\text{ST}} = \epsilon_0 c_0 F^{0\mu}, \quad (29.24)$$

and in particular

$$\Pi_0^{\text{ST}} = 0. \quad (29.25)$$

The fact that the scalar potential has no conjugate momentum is incompatible with the canonical quantization procedure which we wish to impose in a covariant description.

29.1.4 Modified Field Lagrangian Density

We now seek a new Lagrangian density for the free field which is manifestly covariant and which contains the time derivative of the scalar potential. A suitable choice, originally proposed by Fermi, is [155, 178]

$$\mathcal{L}_F = -\frac{\epsilon_0 c_0^2}{2} (\partial_\mu A_\nu) (\partial^\mu A^\nu), \quad (29.26)$$

where summation over μ and ν is implicit. From (29.26) one obtains the conjugate field momenta

$$\Pi_\mu \equiv \frac{\partial \mathcal{L}_F}{\partial \dot{A}_\mu} = -\epsilon_0 \dot{A}_\mu, \quad (29.27)$$

and these are all ($\mu = 0, 1, 2, 3$) nonvanishing.

The Lagrange equations,

$$\sum_{\nu=0}^3 \partial_\nu \left(\frac{\partial \mathcal{L}_F}{\partial (\partial_\nu A_\mu)} \right) - \frac{\partial \mathcal{L}_F}{\partial A_\mu} = 0, \quad (29.28)$$

do not lead to the general form of the field equations, given in (29.12), but to

$$(\partial_\nu \partial^\nu) A^\mu = 0. \quad (29.29)$$

The result in (29.29) is easily derived noting that

$$\frac{\partial \mathcal{L}_F}{\partial A_\mu} = 0, \quad (29.30)$$

and

$$\frac{\partial \mathcal{L}_F}{\partial (\partial_\nu A_\mu)} = -\epsilon_0 c_0^2 \partial^\nu A^\mu. \quad (29.31)$$

The field equations in (29.29) do however agree with those in (29.12) provided

$$\partial_\nu A^\nu = 0. \quad (29.32)$$

A comparison of (29.11) and (29.32) shows that the standard field Lagrangian (29.19) and the modified Lagrangian (29.26) lead to the same result if the Lorenz gauge condition (2.13) is imposed as a subsidiary gauge condition in the modified Lagrangian formalism. In the usual notation the equations in (29.29) are just the free-field Maxwell equations in the Lorenz gauge ((2.14) and (2.15) with $\mathbf{J} = 0$ and $\rho = 0$). We know from the analysis in Sects. 2.2 and 2.3 that the Lorenz condition in (29.32) does not fix the potentials completely. Thus, one obtains from the gauge transformation given by (2.11) and (2.12)

$$\partial_\mu (A')^\mu = \partial_\mu A^\mu - \partial_\mu \partial^\mu \chi. \quad (29.33)$$

Gauge functions χ satisfying $\partial_\mu \partial^\mu \chi = 0$ therefore do not change the Lorenz condition in (29.32).

29.2 Plane-Wave Expansion of the Four-Potential

29.2.1 Four-Component Polarization Vectors

The form of the free-field equations in (29.29) enables us to expand the four-potential in a complete set of plane waves as follows:

$$A^\mu(x) = A^{\mu(+)}(x) + A^{\mu(-)}(x), \quad (29.34)$$

where

$$A^{\mu(+)}(x) = L^{-3/2} \sum_{\mathbf{q}, r} \left(\frac{\hbar}{2\epsilon_0 \omega_{\mathbf{q}}} \right)^{1/2} \epsilon_r^\mu(\mathbf{q}) \alpha_r(\mathbf{q}) e^{-i q_\nu x^\nu}, \quad (29.35)$$

and

$$A^{\mu(-)}(x) = (A^{\mu(+)}(x))^* \quad (29.36)$$

are the positive- and negative-frequency parts of the contravariant potential. The quantities $\alpha_r(\mathbf{q})$ are the actual expansion coefficients. For what follows, it may be helpful to remind the reader of the wave four-vector notation:

$$\{q^\mu\} = (q^0, \mathbf{q}) = (c_0^{-1} \omega_{\mathbf{q}}, \mathbf{q}) = (q, \mathbf{q}), \quad (29.37)$$

and thus

$$\{q_\mu\} = (q_0, -\mathbf{q}) = (c_0^{-1} \omega_{\mathbf{q}}, -\mathbf{q}) = (q, -\mathbf{q}). \quad (29.38)$$

For a massless particle the length of the wave four-vector is zero,

$$q_\mu q^\mu = q_0^2 - \mathbf{q} \cdot \mathbf{q} = 0. \quad (29.39)$$

That $A^{\mu(+)}(x)$ is the positive-frequency part of the potential follows readily if one presents the phase of the exponential function in (29.35) in standard form, i.e.,

$$q x \equiv q_\mu x^\mu = \omega_{\mathbf{q}} t - \mathbf{q} \cdot \mathbf{r}. \quad (29.40)$$

The r -summation in (29.35) runs over four values $r = 0, 1, 2, 3$, due to the fact that for each $\mathbf{q}$ -component of the four-vector potential, $\{A^\mu(x)\}$, there exists four linearly independent polarization vectors $\{\epsilon_r^\mu(\mathbf{q})\}$, which we choose to be real. The polarization vectors satisfy orthonormality and completeness relations, viz.,

$$\epsilon_{r\mu}(\mathbf{q}) \epsilon_s^\mu(\mathbf{q}) = \zeta_r \delta_{rs}, \quad r, s = 0, 1, 2, 3, \quad (29.41)$$

where

$$\zeta_0 = 1, \quad \zeta_1 = \zeta_2 = \zeta_3 = -1, \quad (29.42)$$

and

$$\sum_{r=0}^3 \zeta_r \epsilon_r^\mu(\mathbf{q}) \epsilon_r^\nu(\mathbf{q}) = g^{\mu\nu}. \quad (29.43)$$

Although for many purposes only the general properties in (29.41) and (29.43) are needed, it is useful for the understanding of the covariant field theory's relation to near-field electrodynamics to make a specific choice of polarization vectors. Here, we choose these vectors as follows:

$$\{\epsilon_0^\mu\} = (1, \mathbf{0}) \equiv \{\eta^\mu\}, \quad (29.44)$$

and

$$\{\epsilon_r^\mu(\mathbf{q})\} = (0, \boldsymbol{\epsilon}_r(\mathbf{q})), \quad r = 1, 2, 3. \quad (29.45)$$

The unit vector $\{\epsilon_0^\mu\}$ is the so-called scalar or time-like polarization vector. The other three unit vectors $\{\epsilon_r^\mu\}$, $r = 1, 2, 3$ are named space-like polarization vectors. These vectors are mutually orthogonal, i.e.,

$$\boldsymbol{\epsilon}_r(\mathbf{q}) \cdot \boldsymbol{\epsilon}_s(\mathbf{q}) = \delta_{rs}, \quad r, s = 1, 2, 3, \quad (29.46)$$

and the one ($r = 3$) is directed along $\mathbf{q}$ ($\boldsymbol{\kappa} \equiv \mathbf{q}/q$)

$$\boldsymbol{\epsilon}_3(\mathbf{q}) = \boldsymbol{\kappa} \quad (29.47)$$

and therefore $\{\epsilon_3^\mu\} = (0, \boldsymbol{\kappa})$ is called the longitudinal polarization vector. The remaining two $\{\epsilon_1^\mu\}$ and $\{\epsilon_2^\mu\}$ in analogy with this are called the transverse polarization vectors. With the choice

$$\boldsymbol{\epsilon}_1(\mathbf{q}) \times \boldsymbol{\epsilon}_2(\mathbf{q}) = \boldsymbol{\kappa} \quad (29.48)$$

the vectors $\boldsymbol{\epsilon}_1$, $\boldsymbol{\epsilon}_2$, and $\hat{\mathbf{q}}$ (in this order) form a right-handed set. The choice made for $\{\epsilon_r^\mu\}$, $r = 0, 1, 2, 3$, relates the space-like polarizations directly to the three-vector polarizations given in (15.49)–(15.51). It should be clear for the reader that the specific choice of unit polarization vectors made in (29.44) and (29.45) refers to a given inertial frame.

29.2.2 Gauge, Near-Field, and Transverse Four-Component Potentials

Let us now discuss how we make the bridge between the covariant potential description and the gauge and near-field photon concepts in wave mechanics (Sect. 16.4). The goal thus is to obtain a division of the four-vector potential,

$$\{A^\mu(x)\} = \{A_{T1}^\mu(x)\} + \{A_{T2}^\mu(x)\} + \{A_G^\mu(x)\} + \{A_{NF}^\mu(x)\}, \quad (29.49)$$

into transverse (T1, T2), gauge (G), and near-field (NF) parts. With the specific choice given for the polarization vectors in (29.44) and (29.45) we have

$$\sum_r \epsilon_r^\mu(\mathbf{q}) \alpha_r(\mathbf{q}) = \epsilon_1^\mu \alpha_1 + \epsilon_2^\mu \alpha_2 + \eta^\mu \alpha_0 + \kappa^\mu \alpha_L, \quad (29.50)$$

where $\{\kappa^\mu\} \equiv (0, \kappa)$. The expansion coefficients for the time- and space-like components are in (29.50) denoted by α_0 and α_L , respectively, and the subscript L of course refers to the “longitudinal” character of κ^μ . When the expansion in (29.50) is used in (29.34), the first two terms, $\epsilon_1^\mu \alpha_1$ and $\epsilon_2^\mu \alpha_2$, obviously lead to the two transverse parts ($A_{T1}^\mu(x)$, $A_{T2}^\mu(x)$) of the four-vector potential in (29.49). The expansion coefficients α_G and α_{NF} which relate to the gauge and near-field parts of the four-potential are introduced by a unitary transformation identical to the one in (16.121). Thus,

$$\alpha_L = \frac{1}{\sqrt{2}}(\alpha_G - i\alpha_{NF}), \quad (29.51)$$

$$\alpha_0 = \frac{1}{\sqrt{2}}(\alpha_G + i\alpha_{NF}) \quad (29.52)$$

in analogy with (16.123) and (16.124). Since the α ’s above refer to the positive-frequency parts of the potential a superscript (+) could have been added to these coefficients. For brevity, we omit doing this. The transformations in (29.51) and (29.52) now allow us to express the sum of the last two terms in (29.50) as a function of α_G and α_d :

$$\eta^\mu \alpha_0 + \kappa^\mu \alpha_L = \frac{1}{\sqrt{2}}(\eta^\mu + \kappa^\mu)\alpha_G + \frac{i}{\sqrt{2}}(\eta^\mu - \kappa^\mu)\alpha_{NF}. \quad (29.53)$$

The transformations given for $\mu = 1, 2, 3$ in (29.53) look particularly simple when gathered in vector form. From (29.46)–(29.48) one obtains

$$\{\eta^\mu\} + \{\kappa^\mu\} = (1, \mathbf{0}) + (0, \kappa) = \frac{1}{q}(q, \mathbf{q}) = \frac{1}{q}\{q^\mu\}, \quad (29.54)$$

and of course

$$\{\eta^\mu\} - \{\kappa^\mu\} = \frac{1}{q}\{q_\mu\}, \quad (29.55)$$

and therefore

$$\{\eta^\mu\}\alpha_0 + \{\kappa^\mu\}\alpha_L = \frac{1}{q\sqrt{2}}(\{q^\mu\}\alpha_G + i\{q_\mu\}\alpha_{NF}). \quad (29.56)$$

The relation in (29.56) leads to the following temporary results for the gauge and near-field parts of the positive frequency four-vector potential:

$$\{A_G^{\mu(+)}(x)\} = L^{-3/2} \sum_q \left(\frac{\hbar}{\epsilon_0 \omega_q} \right)^{1/2} \frac{1}{2q} \{q^\mu\} \alpha_G(\mathbf{q}) e^{-iq_\nu x^\nu}, \quad (29.57)$$

and

$$\{A_{\text{NF}}^{\mu(+)}(x)\} = L^{-3/2} \sum_q i \left(\frac{\hbar}{\epsilon_0 \omega_q} \right)^{1/2} \frac{1}{2q} \{q_\mu\} \alpha_{\text{NF}}(\mathbf{q}) e^{-iq_\nu x^\nu}. \quad (29.58)$$

29.2.3 Lorenz Condition: Gauge Arbitrariness

Up to this point we have considered the vector and scalar potentials as independent quantities, but we know from the discussion in Sect. 29.1.4 that the subsidiary Lorenz condition, given in (29.32), leads to a coupling between the scalar potential and the longitudinal part of the vector potential. Using the expansion in (29.35) it is not difficult to show that the Lorenz condition in (29.32) is synonymous with the constraint

$$\sum_{r=0}^3 q_\mu \epsilon_r^\mu(\mathbf{q}) \alpha_r(\mathbf{q}) = 0, \quad (29.59)$$

with the summation convention in force. Since

$$q_\mu \epsilon_r^\mu(\mathbf{q}) = 0, \quad r = 1, 2, \quad (29.60)$$

for the two “transverse” polarization states, (29.59) is reduced to

$$q_\mu \eta^\mu \alpha_0 + q_\mu \kappa^\mu \alpha_L = 0. \quad (29.61)$$

Because $q_\mu \eta^\mu = q$ and $q_\mu \kappa^\mu = -q$, one finally sees that the Lorenz condition implies that the longitudinal and scalar photon expansion coefficients must be equal for every value of $\mathbf{q}$, i.e.,

$$\alpha_0(\mathbf{q}) = \alpha_L(\mathbf{q}). \quad (29.62)$$

In the language of photon wave mechanics this result is the reason that the wave functions of the longitudinal and scalar photons are identical in free space. On the basis of (29.62) one can conclude that

$$\alpha_{\text{NF}}(\mathbf{q}) = 0, \quad \forall \mathbf{q}, \quad (29.63)$$

and in free space the near-field part of the four-vector potential therefore vanishes in every space–time point, i.e.,

$$\{A_{\text{NF}}^\mu(x)\} = 0. \quad (29.64)$$

We know from the analysis in Sect. 16.4.4 that the gauge photon can be eliminated by a gauge transformation within the Lorenz gauge. Consistency with this finding requires that the expression for $\{A_G^{\mu(x)}\}$ in (29.57) must have the structure of a gauge term. In order to prove this one makes use of the relation

$$\partial^\mu \exp(-iq^\nu x_\nu) = -iq^\mu \exp(-iq^\nu x_\nu) \quad (29.65)$$

in (29.57). Since the ∂^μ -operator acts only on the space-time four-vector we immediately obtain

$$A_G^{\mu(+)}(x) = \partial^\mu f^{(+)}(x), \quad (29.66)$$

where

$$f^{(+)}(x) = L^{-3/2} \sum_q \left(\frac{\hbar}{\epsilon_0 \omega_q} \right)^{1/2} \frac{i}{2q} \alpha_G(\mathbf{q}) e^{-iq^\nu x_\nu}. \quad (29.67)$$

On the basis of (29.39) it appears that $f^{(+)}(x)$ satisfies the equation

$$\partial_\mu \partial^\mu f^{(+)}(x) = 0. \quad (29.68)$$

Thus, $A_G^{\mu(+)}(x)$ has the structure of a gauge term, and this also holds for the entire G-part, $\{A_G^\mu(x)\}$. With $f(x) \equiv f^{(+)}(x) + c.c.$, one has from (29.66)

$$A_G^\mu(x) = \partial^\mu f(x). \quad (29.69)$$

For a given nonvanishing $A_G^\mu(x)$ -potential, a gauge transformation

$$A_G^\mu(x) \rightarrow [A_G^\mu(x)]_{\text{NEW}} = \partial^\mu (f(x) - \chi(x)) \quad (29.70)$$

with a gauge function $\chi(x) = f(x)$ enables one to eliminate the new G-potential.

29.2.4 Electromagnetic Field Hamiltonian

To make preparations for the covariant quantization of the electromagnetic field, we now consider the free-field Hamiltonian associated with the modified field Lagrangian density in (29.26). On the basis of the general expression for the Hamiltonian field density, namely

$$\mathcal{H}_F(x) = \Pi_\mu \dot{A}^\mu + \frac{\epsilon_0 c_0^2}{2} (\partial_\mu A_\nu) (\partial^\mu A^\nu), \quad (29.71)$$

and (29.27) for the conjugate field momenta one obtains

$$\mathcal{H}_F(x) = -\epsilon_0 \dot{A}_\mu \dot{A}^\mu + \frac{\epsilon_0 c_0^2}{2} (\partial_\mu A_\nu) (\partial^\mu A^\nu). \quad (29.72)$$

In the usual notation $\mathcal{H}_F$ takes the form

$$\mathcal{H}_F(\mathbf{r}, t) = \frac{\epsilon_0}{2} \left[\dot{\mathbf{A}}^2 - c_0^{-2} \dot{\phi}^2 + c_0^2 \sum_{i,j} (\partial_i A_j)^2 - (\nabla \phi)^2 \right], \quad (29.73)$$

as the reader may verify by means of (29.5) and (29.7). If one uses the relation

$$\sum_{i,j} (\partial_i A_j)^2 = \sum_j (\nabla A_j) \cdot (\nabla A_j), \quad (29.74)$$

the Hamiltonian density can be written in the more symmetric form

$$\mathcal{H}_F(\mathbf{r}, t) = \frac{\epsilon_0}{2} \left\{ \sum_{i=1}^3 [\dot{A}_i^2 + c_0^2 (\nabla A_i)^2] - \dot{A}_0^2 - c_0^2 (\nabla A_0)^2 \right\}. \quad (29.75)$$

Returning to the covariant notation we thus have

$$\begin{aligned} \mathcal{H}_F(x) &= \frac{\epsilon_0}{2} \sum_{\mu=0}^3 (-\zeta_\mu) [(\dot{A}^\mu)^2 + c_0^2 (\nabla A^\mu)^2] \\ &= \frac{\epsilon_0 c_0^2}{2} \sum_{\mu, \nu} (-\zeta_\mu) (\partial_\mu A_\nu) (\partial^\mu A^\nu). \end{aligned} \quad (29.76)$$

where the ζ_μ 's are given in (29.42).

The field Hamiltonian H_F is obtained by integration of $\mathcal{H}_F$ over the direct space, i.e.,

$$H_F = \int_{-\infty}^{\infty} \mathcal{H}_F(\mathbf{r}, t) d^3 r. \quad (29.77)$$

The form in (29.76) in combination with the Parseval–Plancherel relation (9.56) enable one to express H_F as an integral over reciprocal space. Hence,

$$H_F = \frac{\epsilon_0}{2} \sum_{\mu=0}^3 (-\zeta_\mu) \int_{-\infty}^{\infty} [|\dot{A}^\mu(\mathbf{q}; t)|^2 + c_0^2 (i\mathbf{q}) \cdot (-i\mathbf{q}) |A^\mu(\mathbf{q}; t)|^2] \frac{d^3 q}{(2\pi)^3}, \quad (29.78)$$

and then

$$H_F = \frac{\epsilon_0}{2} \sum_{\mu=0}^3 (-\zeta_\mu) \int_{-\infty}^{\infty} [\omega_q^2 |A^\mu(\mathbf{q}; t)|^2 + |\dot{A}^\mu(\mathbf{q}; t)|^2] \frac{d^3 q}{(2\pi)^3}. \quad (29.79)$$

From the continuum version of (29.35) it is clear that

$$\dot{A}^\mu(\mathbf{q}; t) = i\omega_q (A^{\mu(-)}(\mathbf{q}; t) - A^{\mu(+)}(\mathbf{q}; t)), \quad (29.80)$$

and this result enables one to reduce the integrand in (29.79) to the form

$$\omega_q^2 |A^\mu|^2 + |\dot{A}^\mu|^2 = 4\omega_q^2 |A^{\mu(+)}|^2. \quad (29.81)$$

Since

$$\sum_{\mu} \zeta_{\mu} \epsilon_r^{\mu} \epsilon_{r'}^{\mu} = \zeta_r \delta_{rr'}, \quad (29.82)$$

cf. (29.41), it appears from the continuum limit of (29.35) that

$$|A^{\mu}(\mathbf{q}; t)|^2 = \frac{\hbar}{2\epsilon_0\omega_q} \sum_r (-\zeta_r) |\alpha_r(\mathbf{q})|^2, \quad (29.83)$$

and this connection finally leads to the following expression for the free-field Hamiltonian:

$$H_F = \sum_r \int_{-\infty}^{\infty} (-\zeta_r) \hbar \omega_q |\alpha_r(\mathbf{q})|^2 \frac{d^3q}{(2\pi)^3}. \quad (29.84)$$

Up to this point we have assumed that the electromagnetic field possesses a continuous infinity of degrees of freedom. In the discrete-mode case, which corresponds to the mode expansion in (29.35), the field Hamiltonian is given by

$$H_F = \sum_{q,r} (-\zeta_r) \hbar \omega_q |\alpha_r(\mathbf{q})|^2. \quad (29.85)$$

A division of H_F into transverse (T1, T2), longitudinal (L), and scalar (0) parts reads

$$H_F = \sum_q \hbar \omega_q (|\alpha_{T1}(\mathbf{q})|^2 + |\alpha_{T2}(\mathbf{q})|^2 + |\alpha_L(\mathbf{q})|^2 - |\alpha_0(\mathbf{q})|^2). \quad (29.86)$$

Although it seems that the field energy can be negative for some values of the normal variables, this is not so because the subsidiary (Lorenz) condition gives for all physical states $\alpha_L(\mathbf{q}) = \alpha_0(\mathbf{q})$. In free space only the transverse modes contribute to H_F , as we already knew. This can be underlined by expressing α_L and α_0 as functions of α_G and α_{NF} by means of (29.51) and (29.52). Hence, H_F takes the form

$$H_F = \sum_q \hbar \omega_q [|\alpha_{T1}(\mathbf{q})|^2 + |\alpha_{T2}(\mathbf{q})|^2 + i (\alpha_{NF}^*(\mathbf{q}) \alpha_G(\mathbf{q}) - \alpha_{NF}(\mathbf{q}) \alpha_G^*(\mathbf{q}))]. \quad (29.87)$$

Since $\alpha_{NF}(\mathbf{q}) = 0$ (29.62), the gauge potential does not contribute to H_F in free space.

29.3 Covariant Field Quantization

29.3.1 Hamilton Operator and Commutator Relations

The classical field Hamiltonian in (29.85) appears as a sum of energies of a set of fictitious harmonic oscillators, yet with a minus sign on all the scalar field oscillators. Starting from the symmetric form

$$H_F = \sum_{q,r} (-\zeta_r) \frac{1}{2} \hbar \omega_q \left(\alpha_r^*(q) \alpha_r(q) + \alpha_r(q) \alpha_r^*(q) \right), \quad (29.88)$$

the formalism is extended to the quantum level by replacing the normal variables $\alpha_r(q)$ and $\alpha_r^*(q)$ by the annihilation and creation operators $\hat{a}_r(q)$ and $\hat{a}_r^\dagger(q)$ [376]:

$$\alpha_r(q) \rightarrow \hat{a}_r(q), \quad \alpha_r^*(q) \rightarrow \hat{a}_r^\dagger(q). \quad (29.89)$$

To reach the photon interpretation of the quantum fields we require that these operators satisfy the commutation relations

$$[\hat{a}_r(q), \hat{a}_s^\dagger(q')] = -\zeta_r \delta_{rs} \delta_{qq'}, \quad (29.90)$$

$$[\hat{a}_r(q), \hat{a}_s(q')] = [\hat{a}_r^\dagger(q), \hat{a}_s^\dagger(q')] = 0. \quad (29.91)$$

For $r = 1, 2, 3$ ($\zeta_r = -1$) (29.90) and (29.91) are the standard boson commutation relations, but for $r = 0$ ($\zeta_0 = +1$) it looks as if the roles of annihilation ($\hat{a}_0(q)$) and creation ($\hat{a}_0^\dagger(q)$) must be interchanged. Heavy difficulties arise in the formalism if this is done, however. The difficulties which arise from the minus sign for $r = 0$ can be overcome via covariant quantization with an indefinite metric; see Sect. 29.4. The set of annihilation operators related to $r = 1, 2, 3$, for instance, can be those of the two transverse modes ($r = 1, 2$) and the longitudinal mode ($r = 3$) or the set of Cartesian operators ($\hat{a}_x, \hat{a}_y, \hat{a}_z$). As we have seen by an example in Sect. 26.1, an orthogonal transformation ((26.8) and (26.9)) connects the two sets of operators. The Cartesian operator choice allows one to write (29.90) in a partly covariant notation, viz.,

$$[\hat{a}_\mu(q), \hat{a}_\nu^\dagger(q')] = -g_{\mu\nu} \delta_{qq'}. \quad (29.92)$$

The replacements in (29.89) turn the classical field Hamiltonian in (29.85) into the Hamilton operator

$$\hat{H}_F = \sum_{q,r} (-\zeta_r) \frac{1}{2} \hbar \omega_q \left(\hat{a}_r^\dagger(q) \hat{a}_r(q) + \hat{a}_r(q) \hat{a}_r^\dagger(q) \right), \quad (29.93)$$

and by utilizing the commutation relations in (29.90) one finally may write $\hat{H}_F$ in the form

$$\hat{H}_F = \sum_{q,r} \hbar \omega \left(-\zeta_r \hat{a}_r^\dagger(q) \hat{a}_r(q) + \frac{1}{2} \right). \quad (29.94)$$

At this point, I urge the reader to convince himself that the covariant momentum–energy operator of the field can be written in (partly) covariant notation as

$$\{\hat{P}_{F,\mu}\} = - \sum_q \frac{1}{2} \hbar \{q_\mu\} \sum_{\nu,\rho} g^{\nu\rho} \left(\hat{a}_\nu^\dagger \hat{a}_\rho + \hat{a}_\rho \hat{a}_\nu^\dagger \right). \quad (29.95)$$

In the following, the part of the field Hamilton operator which contains the longitudinal and scalar modes is of particular interest. Therefore, we divide $\hat{H}_F$ into three pieces:

$$\hat{H}_F = \hat{H}_F^T + \hat{H}_F^{LS} + \frac{1}{2} \sum_{q,r} \hbar \omega_q, \quad (29.96)$$

where

$$\hat{H}_F^T = \sum_q \hbar \omega_q \left(\hat{a}_{T1}^\dagger(\mathbf{q}) \hat{a}_{T1}(\mathbf{q}) + \hat{a}_{T2}^\dagger(\mathbf{q}) \hat{a}_{T2}(\mathbf{q}) \right) \quad (29.97)$$

gives the contributions from the transverse modes, and

$$\hat{H}_F^{LS} = \sum_q \hbar \omega_q \left(\hat{a}_L^\dagger(\mathbf{q}) \hat{a}_L(\mathbf{q}) - \hat{a}_0^\dagger(\mathbf{q}) \hat{a}_0(\mathbf{q}) \right) \quad (29.98)$$

contains the contributions from the longitudinal and scalar modes. The last term in (29.96), as we know, represents the (infinite) energy of the photon vacuum.

29.3.2 Scalar Photons: The Problem of Negative Norms

The global vacuum state of the field, $|0\rangle$, is the state in which there are no photons of any kind present. The vacuum state thus satisfies for all $\mathbf{q}$

$$\hat{a}_r(\mathbf{q})|0\rangle = 0, \quad r = 0, 1, 2, 3. \quad (29.99)$$

A one-photon state, $|1_r(\mathbf{q})\rangle$, belonging to the mode $(\mathbf{q}, r)$ is obtained by acting with the operator $\hat{a}_r^\dagger(\mathbf{q})$ on the vacuum state, i.e.,

$$|1_r(\mathbf{q})\rangle = \hat{a}_r^\dagger(\mathbf{q})|0\rangle. \quad (29.100)$$

The form given for $\hat{H}_F$ in (29.94) suggests that one introduces the photon number operator belonging to the mode $(\mathbf{q}, r)$ by the definition

$$\hat{N}_r(\mathbf{q}) \equiv -\zeta_r \hat{a}_r^\dagger(\mathbf{q}) \hat{a}_r(\mathbf{q}). \quad (29.101)$$

By utilizing the commutation relation in (29.90) we obtain

$$\begin{aligned} \sum_{k,s} \hbar \omega_k \hat{N}_s(\mathbf{k}) |1_r(\mathbf{q})\rangle &= \sum_{k,s} \hbar \omega_k (-\zeta_s) \hat{a}_s^\dagger(\mathbf{k}) \hat{a}_s(\mathbf{k}) \hat{a}_r^\dagger(\mathbf{q}) |0\rangle \\ &= \hbar \omega_q \hat{a}_r^\dagger(\mathbf{q}) |0\rangle = \hbar \omega_q |1_r(\mathbf{q})\rangle, \end{aligned} \quad (29.102)$$

and this means that the one-photon energy has the *positive* value $\hbar \omega_q$ for transverse, longitudinal and scalar photons. Despite of the minus sign ($-\zeta_0 = -1$) associated with the scalar photons in (29.94), these photons do have positive energy in our description.

Although the formalism up to this point seems satisfactory, there are some difficulties related to the norms of the scalar photon states. To show this, let us consider the relation between the norms of neighboring number states. Since the n -photon state $|n_r(\mathbf{q})\rangle$ can be generated from the ground state via

$$|n_r(\mathbf{q})\rangle = \frac{1}{\sqrt{n_r(\mathbf{q})!}} \left(\hat{a}_r^\dagger(\mathbf{q}) \right)^{n_r(\mathbf{q})} |0\rangle, \quad (29.103)$$

cf. (23.67), one has

$$\begin{aligned} n_r(\mathbf{q}) \langle n_r(\mathbf{q}) | n_r(\mathbf{q}) \rangle &= \langle n_r(\mathbf{q}) - 1 | \hat{a}_r(\mathbf{q}) \hat{a}_r^\dagger(\mathbf{q}) | n_r(\mathbf{q}) - 1 \rangle \\ &= \langle n_r(\mathbf{q}) - 1 | \hat{a}_r^\dagger(\mathbf{q}) \hat{a}_r(\mathbf{q}) - \zeta_r | n_r(\mathbf{q}) - 1 \rangle. \end{aligned} \quad (29.104)$$

From (29.101) we find

$$\hat{a}_r^\dagger(\mathbf{q}) \hat{a}_r(\mathbf{q}) = -\zeta_r \hat{N}_r(\mathbf{q}), \quad (29.105)$$

and when this relation is inserted into (29.104), it is easy to show that

$$\langle n_r(\mathbf{q}) | n_r(\mathbf{q}) \rangle = -\zeta_r \langle n_r(\mathbf{q}) - 1 | n_r(\mathbf{q}) - 1 \rangle. \quad (29.106)$$

Starting from a normalized ground state, i.e.,

$$\langle 0 | 0 \rangle = 1, \quad (29.107)$$

it appears from (29.106) that for any state containing an odd number of scalar photons the norm will be negative. For transverse and longitudinal photon number states the norms are always positive. At first sight the appearance of negative norms seems to be serious problem because the probability interpretation of quantum physics requires that the states have positive norms. However, we must remember that our quantized formalism not yet is equivalent to the quantized Maxwell theory since we up to now have ignored the constraint imposed by the Lorenz condition. In the classical description the negative sign in front of $|\alpha_0|^2$ in the Hamiltonian (29.85) causes no problems because the Lorenz condition requires that the expansion coefficients for the longitudinal and scalar fields must be equal for all physical free-field states, see (29.62).

29.3.3 Gupta–Bleuler–Lorenz Condition

*** We must now try to built-in the Lorenz condition [150–152] in our quantum mechanical treatment. Unfortunately, one cannot take the Lorenz condition (29.32) as an operator identity. To understand this let us consider the operator

$$\partial_\mu \hat{A}^\mu(x) = \partial_\mu \hat{A}^{\mu(+)}(x) + h.c., \quad (29.108)$$

where, by the first replacement in (29.89), one has from (29.35) the operator expansion

$$\hat{A}^{\mu(+)}(x) = L^{-3/2} \sum_{\mathbf{q}, r} \left(\frac{\hbar}{2\epsilon_0 \omega_{\mathbf{q}}} \right)^{1/2} \epsilon_r^\mu(\mathbf{q}) \hat{a}_r(\mathbf{q}) e^{-i q_\nu x^\nu}. \quad (29.109)$$

With the choice of polarization vectors given in (29.44) and (29.45) one obtains

$$\sum_{r=0}^3 q_\mu \epsilon_r^\mu(\mathbf{q}) \hat{a}_r(\mathbf{q}) = q (\hat{a}_0(\mathbf{q}) - \hat{a}_L(\mathbf{q})), \quad (29.110)$$

and with the help of this relation the reader may show that

$$\partial_\mu \hat{A}^{\mu(+)}(x) = i L^{-3/2} \sum_{\mathbf{q}} \left(\frac{\hbar \omega_{\mathbf{q}}}{2\epsilon_0 c_0^2} \right)^{1/2} (\hat{a}_L(\mathbf{q}) - \hat{a}_0(\mathbf{q})) e^{-i q_\nu x^\nu}. \quad (29.111)$$

Since the operators $\hat{a}_L(\mathbf{q})$ and $\hat{a}_0(\mathbf{q})$ act in different subspaces of the state space, viz., the subspaces of the longitudinal and scalar photons, the operator $\partial_\mu \hat{A}^{\mu(+)}(x)$ cannot be identically zero.

A satisfactory solution to the problem was given by Gupta [314] and Bleuler [315] who suggested to use a subsidiary condition of the form

$$\partial_\mu \hat{A}^{\mu(+)}(x) |\psi\rangle = 0. \quad (29.112)$$

The condition in (29.112) involves absorption operators only, and it appears from (29.111) that the Gupta–Bleuler–Lorenz condition is satisfied in all space–time points if

$$(\hat{a}_L(\mathbf{q}) - \hat{a}_0(\mathbf{q})) |\psi\rangle = 0 \quad (29.113)$$

for all $\mathbf{q}$. We shall not here discuss the possibilities of making other choices for the subsidiary condition. If the quantized electromagnetic field is coupled to a matter field the condition in (29.113) must be generalized because the annihilation operator $\hat{a}_\mu(\mathbf{q})$ no longer satisfies the free evolution equation

$$\frac{d}{dt} \hat{a}_\mu(\mathbf{q}) = \frac{1}{i\hbar} [\hat{a}_\mu(\mathbf{q}), \hat{H}_F]. \quad (29.114)$$

From (29.112) and its adjoint

$$\langle \psi | \partial_\mu \hat{A}^{\mu(-)}(x) = 0 \quad (29.115)$$

it follows that the Lorenz condition holds for the quantum mechanical mean value, i.e.,

$$\langle \psi | \partial_\mu \hat{A}^\mu(x) | \psi \rangle = 0, \quad \forall x. \quad (29.116)$$

This result ensures that the theory becomes correct in the classical limit.

In free space the longitudinal and scalar photons cannot contribute to the mean value of the field energy, or of any other field observables. To show this for $\hat{H}_F$, we consider

$$\langle \psi | \hat{H}_F^{\text{LS}} | \psi \rangle = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \langle \psi | \hat{a}_{\text{L}}^{\dagger}(\mathbf{q}) \hat{a}_{\text{L}}(\mathbf{q}) - \hat{a}_0^{\dagger}(\mathbf{q}) \hat{a}_0(\mathbf{q}) | \psi \rangle. \quad (29.117)$$

By means of the adjoint of (29.113), viz.,

$$\langle \psi | (\hat{a}_{\text{L}}^{\dagger}(\mathbf{q}) - \hat{a}_0^{\dagger}(\mathbf{q})) = 0, \quad (29.118)$$

one obtains

$$\langle \psi | \hat{a}_{\text{L}}^{\dagger}(\mathbf{q}) \hat{a}_{\text{L}}(\mathbf{q}) - \hat{a}_0^{\dagger}(\mathbf{q}) \hat{a}_0(\mathbf{q}) | \psi \rangle = \langle \psi | \hat{a}_{\text{L}}^{\dagger}(\mathbf{q}) (\hat{a}_{\text{L}}(\mathbf{q}) - \hat{a}_0(\mathbf{q})) | \psi \rangle = 0, \quad (29.119)$$

where the last member of (29.119) follows from the subsidiary condition in (29.113). From the result in (29.119) it is clear that

$$\langle \psi | \hat{H}_F^{\text{LS}} | \psi \rangle = 0, \quad (29.120)$$

and hence

$$\langle \psi | \hat{H}_F | \psi \rangle = \langle \psi | \hat{H}_F^{\text{T}} | \psi \rangle, \quad (29.121)$$

i.e., only transverse photons can contribute to the mean value of the field energy as a consequence of the Gupta–Bleuler–Lorenz condition.

29.3.4 Near-Field and Gauge Photon Quanta: Commutators and Hamilton Operator

The extension of the classical theory to the quantum level via the replacements in (29.89) in combination with the relations given in (29.51) and (29.52), suggest that the normal variables $\alpha_G(\mathbf{q})$ and $\alpha_{\text{NF}}(\mathbf{q})$ of the gauge field and near field are extended to the quantum level as follows:

$$\hat{a}_G(\mathbf{q}) = \frac{1}{\sqrt{2}} (\hat{a}_{\text{L}}(\mathbf{q}) + \hat{a}_0(\mathbf{q})), \quad (29.122)$$

$$\hat{a}_{\text{NF}}(\mathbf{q}) = \frac{i}{\sqrt{2}} (\hat{a}_{\text{L}}(\mathbf{q}) - \hat{a}_0(\mathbf{q})). \quad (29.123)$$

Associated with these annihilation operators, we have the creation operators

$$\hat{a}_G^\dagger(\mathbf{q}) = \frac{1}{\sqrt{2}} \left(\hat{a}_L^\dagger(\mathbf{q}) + \hat{a}_0^\dagger(\mathbf{q}) \right), \quad (29.124)$$

$$\hat{a}_{\text{NF}}^\dagger(\mathbf{q}) = \frac{i}{\sqrt{2}} \left(\hat{a}_0^\dagger(\mathbf{q}) - \hat{a}_L^\dagger(\mathbf{q}) \right). \quad (29.125)$$

By means of the commutation relations in (29.90) and (29.91) for the longitudinal ($r = 3$) and scalar ($r = 0$) photons, it is easy to see that the annihilation and creation operators of the gauge and near-field photons satisfy the following set of commutation relations:

$$\left[\hat{a}_G(\mathbf{q}), \hat{a}_G^\dagger(\mathbf{q}') \right] = \left[\hat{a}_{\text{NF}}(\mathbf{q}), \hat{a}_{\text{NF}}^\dagger(\mathbf{q}') \right] = 0, \quad (29.126)$$

$$\left[\hat{a}_G(\mathbf{q}), \hat{a}_G^\dagger(\mathbf{q}') \right] = \left[\hat{a}_G^\dagger(\mathbf{q}), \hat{a}_G^\dagger(\mathbf{q}') \right] = 0, \quad (29.127)$$

$$\left[\hat{a}_{\text{NF}}(\mathbf{q}), \hat{a}_{\text{NF}}^\dagger(\mathbf{q}') \right] = \left[\hat{a}_{\text{NF}}^\dagger(\mathbf{q}), \hat{a}_{\text{NF}}^\dagger(\mathbf{q}') \right] = 0, \quad (29.128)$$

and the cross-coupling relations

$$\left[\hat{a}_{\text{NF}}(\mathbf{q}), \hat{a}_G^\dagger(\mathbf{q}') \right] = i \delta_{\mathbf{q}\mathbf{q}'} \quad (29.129)$$

$$\left[\hat{a}_{\text{NF}}(\mathbf{q}), \hat{a}_G(\mathbf{q}') \right] = \left[\hat{a}_{\text{NF}}^\dagger(\mathbf{q}), \hat{a}_G^\dagger(\mathbf{q}') \right] = 0. \quad (29.130)$$

In order to rewrite the part of the free-field Hamiltonian which contains the contributions from the longitudinal and scalar modes in terms of the annihilation and creation operators of the near-field and gauge photons, one inserts the inverse transformation to the one given in (29.122) and (29.123) into (29.98). This readily leads to the expression

$$\hat{H}_F^{\text{LS}} = i \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \left(\hat{a}_{\text{NF}}^\dagger(\mathbf{q}) \hat{a}_G(\mathbf{q}) - \hat{a}_G^\dagger(\mathbf{q}) \hat{a}_{\text{NF}}(\mathbf{q}) \right) \equiv \hat{H}_F^{\text{NFG}}. \quad (29.131)$$

The result above shows that the Hamilton operator involves a cross-coupling between the G and NF operators. From a physical point of view there is nothing wrong in this, but in a formal sense it would be nice to write the Hamiltonian in a form containing the number operators ($\hat{a}_G^\dagger \hat{a}_G$ and $\hat{a}_{\text{NF}}^\dagger \hat{a}_{\text{NF}}$) for the different modes, and no cross-coupling. The cross-coupling can be traced back to the presence of the minus sign in front of the scalar mode contribution to $\hat{H}_F^{\text{LS}}$; see (29.98). Our formal problem thus originates in the same source as the problem of the negative norms of field states containing an uneven number of scalar photons.

29.4 Covariant Quantization with an Indefinite Metric

29.4.1 New Scalar Product and New Adjoining Operator, $\bar{\mathcal{O}}$

In the present subsection I shall *very* briefly describe a method [178, 236, 314, 315, 322, 323] which solves the “problems” associated with the negative norms and related issues. For brevity, the $\wedge$ -symbol will be omitted on all operators in this and the next subsection.

We start by introducing a so-called linear metric operator M , which is assumed to be both Hermitian and unitary, that is

$$M = M^\dagger = M^{-1}. \quad (29.132)$$

With old kets ($|\psi\rangle$) and bras ($\langle\phi|$) we then associate new ones defined by

$$|\psi \rhd \equiv |\psi\rangle, \quad (29.133)$$

$$\lhd \phi| \equiv \langle\phi|M. \quad (29.134)$$

For the general linear operator $\mathcal{O}$ new matrix elements are introduced as follows

$$\lhd \phi|\mathcal{O}|\psi \rhd \equiv \langle\phi|M\mathcal{O}|\psi\rangle. \quad (29.135)$$

Letting $\mathcal{O}$ be the identity operator, it is clear that the new scalar product ($\phi|\psi$) will be given by

$$\lhd \phi|\psi \rhd = \langle\phi|M|\psi\rangle. \quad (29.136)$$

If one takes (29.136) as the definition of the new scalar product, (29.135) follows as a consequence. The new metric associated with M is called *indefinite* because the norm ($\psi|\psi$) can be negative or zero. Although negative norms at first sight seem to confront us with a serious problem, since the probability interpretation of quantum mechanics requires that states have positive norms, it turns out that *all* predictions about physical variables stay acceptable. It follows from (29.132) and (29.136) that the new scalar product satisfies the relation

$$\lhd \phi|\psi \rhd = \lhd \psi|\phi \rhd^*. \quad (29.137)$$

To the operator $\mathcal{O}$ we now associate a new adjoint (Hermitian conjugate) operator $\bar{\mathcal{O}}$ by the definition

$$\lhd \phi|\bar{\mathcal{O}}|\psi \rhd \equiv \lhd \psi|\mathcal{O}|\phi \rhd^* \quad (29.138)$$

for all ψ and ϕ . The operator $\mathcal{O}$ is Hermitian in the new metric if $\mathcal{O} = \bar{\mathcal{O}}$, and if so, the diagonal elements $\lhd \psi|\mathcal{O}|\psi \rhd$ are real. It appears from (29.137) and (29.138) that one has the following bra-ket connection:

$$|\chi \rhd = \mathcal{O}|\psi \rhd \leftrightarrow \lhd \chi| = \lhd \psi|\bar{\mathcal{O}}. \quad (29.139)$$

For what follows, it is important to determine the relationship between the old ($\mathcal{O}^\dagger$) and new ($\bar{\mathcal{O}}$) adjoints to $\mathcal{O}$. Starting from (29.138), this relationship may easily be obtained using the definitions in (29.133) and (29.134). Hence, the left side of (29.138) becomes

$$\subset \phi | \bar{\mathcal{O}} | \psi \supset = \langle \phi | M \bar{\mathcal{O}} | \psi \rangle, \quad (29.140)$$

and for the right side we get

$$\subset \psi | \mathcal{O} | \phi \supset^* = \langle \psi | M \mathcal{O} | \phi \rangle^* = \langle \phi | \mathcal{O}^\dagger M^\dagger | \psi \rangle. \quad (29.141)$$

A comparison then shows that $M \bar{\mathcal{O}} = \mathcal{O}^\dagger M^\dagger$, and by multiplication of this connection by $M^{-1} = M$ from the left we finally have

$$\bar{\mathcal{O}} = M \mathcal{O}^\dagger M \quad (29.142)$$

since $M^\dagger = M$.

Before ending this brief introduction of the indefinite metric Hilbert space, let me mention that the notion of eigenvector and eigenvalues is independent of the metric because of the definition in (29.133). The closure theorem ((11.14), generalized) takes the form

$$\sum_n |u_n\rangle \supset \subset u_n | M = \hat{1} \quad (29.143)$$

in the new metric, since $\subset u_n | M = \langle u_n | M^2 = \langle u_n |$, the last equality following from (29.132).

29.4.2 Choice of New Metric

In our old (definite metric: $M = \hat{1}$) covariant formalism, the classical four-potential expansion given by (29.34)–(29.36) was extended to the quantum level by the replacements in (29.89). Thus, with omission of the operator symbol $\wedge$,

$$A^\mu(x) = L^{-3/2} \sum_{q,r} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \epsilon_r^\mu(q) \left[a_r(q) e^{-iq_\nu x^\nu} + a_r^\dagger(q) e^{iq_\nu x^\nu} \right]. \quad (29.144)$$

All calculations carried out so far remain valid in the new indefinite metric provided all old adjoints $\mathcal{O}^\dagger$ are replaced by the new ones $\bar{\mathcal{O}}$. This replacement ensures that mean values calculated in the new metric will be real. Thus, the contravariant four-potential operator is given by the plane-wave expansion

$$A^\mu(x) = L^{-3/2} \sum_{q,r} \left(\frac{\hbar}{2\epsilon_0 \omega_q} \right)^{1/2} \epsilon_r^\mu(q) \left[a_r(q) e^{-iq_\nu x^\nu} + \bar{a}_r(q) e^{iq_\nu x^\nu} \right] \quad (29.145)$$

in the new metric, and the annihilation and new creation operators satisfy the commutation relations

$$[a_r(\mathbf{q}), \bar{a}_s(\mathbf{q}')] = -\zeta_r \delta_{rs} \delta_{\mathbf{q}\mathbf{q}'}, \quad (29.146)$$

$$[a_r(\mathbf{q}), a_s(\mathbf{q}')] = [\bar{a}_r(\mathbf{q}), \bar{a}_s(\mathbf{q}')] = 0. \quad (29.147)$$

The free-field Hamilton operator now reads

$$H_F = \sum_{\mathbf{q}, r} \hbar \omega_{\mathbf{q}} \left(-\zeta_r \bar{a}_r(\mathbf{q}) a_r(\mathbf{q}) + \frac{1}{2} \right), \quad (29.148)$$

and there is still a minus sign on the scalar ($r = 0$) oscillator contributions.

Since the problem of the negative norms of the scalar photon states comes from this minus sign, we seek a metric which can correct this, and only this. The metric we look for thus must play an active role only the subspace of the scalar photons. Mathematically phrased, we try to find an M such that

$$\bar{a}_0 = M a_0^\dagger M = -a_0^\dagger, \quad (29.149)$$

while

$$\bar{a}_r = M a_r^\dagger M = a_r^\dagger, \quad r = 1, 2, 3. \quad (29.150)$$

Let us first study the eigenvalues m of M . Since M is Hermitian, the m 's are real. By operating on the eigenvalue equation for M , i.e.,

$$M|m\rangle = m|m\rangle, \quad (29.151)$$

with M , and using that M^2 equals the identity operator, we have

$$|m\rangle = M^2|m\rangle = m^2|m\rangle. \quad (29.152)$$

In consequence, the eigenvalues of M necessarily are equal to $+1$ or -1 . The metric operator defined by

$$M|n_0\rangle = (-1)^{n_0}|n_0\rangle \quad (29.153)$$

satisfies our demands. Thus, by a comparison of the expressions

$$M a_0^\dagger |n_0\rangle = (-1)^{n_0+1} \sqrt{n_0+1} |n_0+1\rangle, \quad (29.154)$$

and

$$a_0^\dagger M |n_0\rangle = (-1)^{n_0} \sqrt{n_0+1} |n_0+1\rangle, \quad (29.155)$$

it follows that $M a_0^\dagger = -a_0^\dagger M$ since the set $\{|n_0\rangle\}$ forms a basis in the state space of the scalar photon. By multiplying this relation with M from the right side one obtains precisely (29.149). The new metric associated with M clearly allows states

with negative norms. Hence, (29.153) gives

$$\subset n_0 |n'_0 \supset = \langle n_0 | M | n'_0 \rangle = (-1)^{n_0} \delta_{n_0 n'_0}, \quad (29.156)$$

confirming that states with an uneven number of scalar photons have a negative norm.

By inserting the relations in (29.149) and (29.150) into the commutation relation in (29.146) one obtains

$$\left[a_r(\mathbf{q}), a_s^\dagger(\mathbf{q}') \right] = \delta_{rs} \delta_{\mathbf{q}\mathbf{q}'}. \quad (29.157)$$

In the new metric, a_0 and $a_0^\dagger$, therefore, become normal annihilation and creation operators. Expressed in terms of the old adjoints the field Hamiltonian in (29.148) takes the form

$$H_F = \sum_{\mathbf{q}, r} \hbar \omega_{\mathbf{q}} \left(a_r^\dagger(\mathbf{q}) a_r(\mathbf{q}) + \frac{1}{2} \right), \quad (29.158)$$

i.e., with a “normal” plus sign also on the scalar contribution. The basis states of the individual scalar modes hence are generated by the usual prescription:

$$|n_0\rangle = \frac{1}{\sqrt{n_0!}} (a_0^\dagger)^{n_0} |0_S\rangle \quad (29.159)$$

$|0_S\rangle$ being the scalar-photon vacuum.

29.4.3 Near-Field and Gauge Photons in the New Metric

In the covariant quantization scheme with an indefinite metric the annihilation operators for gauge and near-field photons are still given by (29.122) and (29.123), but the associated creation operators

$$\begin{aligned} \bar{a}_G(\mathbf{q}) &= \frac{1}{\sqrt{2}} (\bar{a}_L(\mathbf{q}) + \bar{a}_0(\mathbf{q})) \\ &= \frac{1}{\sqrt{2}} (a_L^\dagger(\mathbf{q}) - a_0^\dagger(\mathbf{q})), \end{aligned} \quad (29.160)$$

$$\begin{aligned} \bar{a}_{\text{NF}}(\mathbf{q}) &= \frac{i}{\sqrt{2}} (\bar{a}_0(\mathbf{q}) - \bar{a}_L(\mathbf{q})) \\ &= -\frac{i}{\sqrt{2}} (a_L^\dagger(\mathbf{q}) + a_0^\dagger(\mathbf{q})), \end{aligned} \quad (29.161)$$

now come with a minus sign in front of the old creation operator $a_0^\dagger(\mathbf{q})$. In consequence, the commutator relations in (29.126) are replaced by “usual” ones, viz.,

$$\left[a_G(\mathbf{q}), a_G^\dagger(\mathbf{q}') \right] = \left[a_{\text{NF}}(\mathbf{q}), a_{\text{NF}}^\dagger(\mathbf{q}') \right] = \delta_{\mathbf{q}\mathbf{q}'}, \quad (29.162)$$

and the cross-coupling connection in (29.129) by

$$\left[a_{\text{NF}}(\mathbf{q}), a_G^\dagger(\mathbf{q}) \right] = 0. \quad (29.163)$$

Since

$$\bar{a}_{\text{NF}}(\mathbf{q}) = -i a_G^\dagger(\mathbf{q}), \quad (29.164)$$

$$\bar{a}_G(\mathbf{q}) = i a_{\text{NF}}^\dagger(\mathbf{q}), \quad (29.165)$$

as the reader may show, it appears that the Hamiltonian

$$H_F^{\text{NFG}} = i \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} (\bar{a}_{\text{NF}}(\mathbf{q}) a_G(\mathbf{q}) - \bar{a}_G(\mathbf{q}) a_{\text{NF}}(\mathbf{q})), \quad (29.166)$$

being the replacement of (29.131) in our indefinite metric formalism, is given by

$$H_F^{\text{NFG}} = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} \left(a_G^\dagger(\mathbf{q}) a_G(\mathbf{q}) + a_{\text{NF}}^\dagger(\mathbf{q}) a_{\text{NF}}(\mathbf{q}) \right) \quad (29.167)$$

in terms of the old adjoints. In the new description a Fock-state basis for the kets in the combined subspace of the near-field and gauge photons can be constructed in the usual manner. For each value of the mode wave vector we thus have

$$|n_{\text{NF}}, n_G\rangle = \frac{1}{\sqrt{n_{\text{NF}}! n_G!}} (a_{\text{NF}}^\dagger)^{n_{\text{NF}}} (a_G^\dagger)^{n_G} |0\rangle, \quad (29.168)$$

where $|0\rangle = |0_{\text{NF}}, 0_G\rangle$ is the subspace vacuum state. The transformations in (29.122) and (29.123) make it clear that the vacuum of the NF and G photons coincides with that of the L and S photons:

$$|0_{\text{NF}}, 0_G\rangle = |0_{\text{L}}, 0_{\text{S}}\rangle. \quad (29.169)$$

For a *free* field, the Gupta–Bleuler–Lorenz condition in (29.113) must be satisfied. In view of (29.123), the subsidiary condition may be written as

$$a_{\text{NF}}(\mathbf{q})|\psi\rangle = 0, \quad \forall \mathbf{q}. \quad (29.170)$$

In free space, the physical kets therefore have no near-field photons. It follows from (29.170) that

$$a_{\text{NF}}(\mathbf{q})|\psi \supseteq 0 \leftrightarrow \psi | \bar{a}_{\text{NF}}(\mathbf{q}) = 0. \quad (29.171)$$

In consequence, the new mean value of the operator A_{NF}^μ , which is obtained by the replacements $\alpha_{\text{NF}} \rightarrow a_{\text{NF}}$ and $\alpha_{\text{NF}}^* \rightarrow \bar{a}_{\text{NF}}$ in the classical expressions ((29.58), and its complex conjugate) is zero:

$$\frac{\subset \psi | A_{\text{NF}}^\mu | \psi \supset}{\subset \psi | \psi \supset} = 0. \quad (29.172)$$

It is not difficult to show that the mean value of the gauge potential operator, A_G^μ , is given by

$$\frac{\subset \psi | A_G^\mu | \psi \supset}{\subset \psi | \psi \supset} = -\partial^\mu \subset f \supset, \quad (29.173)$$

where $\subset f \supset$ is the new mean value of the gauge function operator. This operator is obtained by the replacement $\alpha_G \rightarrow a_G$ and $\alpha_G^* \rightarrow \bar{a}_G$ in (29.67) and its complex conjugate, respectively. The form of the right side of (29.173) demonstrates that the mean value of A_G^μ has the character of a gauge term.

29.5 $\hat{A}^\mu(x)$ -Commutators and the Feynman Photon Propagator

29.5.1 Covariant Commutation Relations

Starting from the commutation relations between the annihilation and creation operators belonging to the various field modes ((29.90) and (29.91)) one can obtain covariant commutation relations between the components of the four-potential operators, $\{\hat{A}^\mu(x)\}$. Since the positive-frequency part of the four-potential $\hat{A}^{\mu(+)}(x)$, contains only annihilation operators, $\hat{a}_r(\mathbf{q})$, in its expansion (see (29.144)), and the negative-frequency part, $\hat{A}^{\mu(-)}(x)$, only creation operators, $\hat{a}_r^\dagger(\mathbf{q})$, it follows immediately from (29.91) that

$$[\hat{A}^\mu(x), \hat{A}^\nu(x')] = [\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')] + [\hat{A}^{\mu(-)}(x), \hat{A}^{\nu(+)}(x')]. \quad (29.174)$$

The commutators on the right side of this equation are related by

$$[\hat{A}^{\mu(-)}(x), \hat{A}^{\nu(+)}(x')] = -[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')]^\dagger, \quad (29.175)$$

and therefore we may concentrate our efforts on the calculation of just one of these, say $[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')]$. When the mode expansions for $\hat{A}^{\mu(+)}(x)$ and $\hat{A}^{\nu(-)}(x')$ are inserted in the commutator we get a double sum over both wave vectors and polarization indices. The Kronecker delta's δ_{rs} and $\delta_{qq'}$ appearing in (29.90) immediately reduce the double sums to single sums. Hence, one obtains

$$[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')] = \frac{\hbar}{2\epsilon_0 L^3} \sum_{\mathbf{q}, r} (-\zeta_r) \epsilon_r^\mu(\mathbf{q}) \epsilon_r^\nu(\mathbf{q}) e^{-iq_\nu [x^\nu - (x')^\nu]}. \quad (29.176)$$

The summation over the polarization states gives us the metric tensor $g^{\mu\nu}$ (see (29.43)), so that

$$\begin{aligned} \left[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x') \right] &= \frac{\hbar}{2\epsilon_0 L^3} (-g^{\mu\nu}) \sum_q \frac{1}{\omega_q} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\omega_q(t-t')} \\ &\rightarrow -\frac{\hbar}{2\epsilon_0} g^{\mu\nu} \int_{-\infty}^{\infty} \frac{1}{\omega_q} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} e^{-i\omega_q(t-t')} \frac{d^3q}{(2\pi)^3} \end{aligned} \quad (29.177)$$

in the standard notation, and with a transition to the continuum limit. The integral in (29.177) multiplied by $c_0^2/(2i)$ equals the $\Delta^+(x - x')$ -part of the massless Jordan–Pauli scalar propagator; see (24.1). The result

$$\left[\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x') \right] = \frac{i\hbar}{\epsilon_0 c_0^2} (-g^{\mu\nu}) \Delta^+(x - x'), \quad (29.178)$$

together with the relations in (24.3), (24.5), and (29.175), finally lead to the following covariant commutation relations for the four-potential operators $\hat{A}^\mu(x)$:

$$\left[\hat{A}^\mu(x), \hat{A}^\nu(x') \right] = \frac{i\hbar}{\epsilon_0 c_0^2} G^{\mu\nu}(x - x'), \quad (29.179)$$

where

$$G^{\mu\nu}(x) = -g^{\mu\nu} \lim_{m \rightarrow 0} \Delta_{\text{JP}}(x). \quad (29.180)$$

29.5.2 Equal-Time Commutation Relations

From the expression given in (24.10) for the Jordan–Pauli function $\Delta_{\text{JP}}(x) = \Delta_{\text{JP}}(R, \tau)$ it appears that $\Delta_{\text{JP}}(R, 0) = 0$. Thus, one obtains the equal-time commutation relations

$$\left[\hat{A}^\mu(\mathbf{r}, t), \hat{A}^\mu(\mathbf{r}', t) \right] = 0 \quad (29.181)$$

among the various field operators. The conjugate field momentum operators given by

$$\hat{\Pi}^\mu(x) = -\epsilon_0 \frac{\partial}{\partial t} \hat{A}^\mu(x), \quad (29.182)$$

cf. (29.27), in consequence of (29.181) satisfy the equal-time commutation relations

$$\left[\hat{\Pi}^\mu(\mathbf{r}, t), \hat{\Pi}^\nu(\mathbf{r}', t) \right] = 0. \quad (29.183)$$

In order to determine the commutator of $\hat{A}^\mu(\mathbf{r}, t)$ and $\hat{\Pi}^\nu(\mathbf{r}', t)$, let us consider the equal-time commutator

$$\begin{aligned}
[\hat{A}^\mu(\mathbf{r}, t), \frac{\partial}{\partial t} \hat{A}^\nu(\mathbf{r}', t)] &= [\hat{A}^{\mu(+)}(\mathbf{r}, t), \frac{\partial}{\partial t} \hat{A}^{\nu(-)}(\mathbf{r}', t)] \\
&\quad - [\hat{A}^{\mu(+)}(\mathbf{r}, t), \frac{\partial}{\partial t} \hat{A}^{\nu(-)}(\mathbf{r}', t)]^\dagger.
\end{aligned} \tag{29.184}$$

The correctness of the relation above follows from the fact that the annihilation and creation operators of the individual field modes are time independent here. The structures of the commutators in (29.174) and (29.184) therefore must be analogues. The first commutator on the right side of (29.184) may be obtained by differentiating (29.177) with respect to t' , and thereafter setting $t' = t$. Hence, we find in the continuum limit

$$\begin{aligned}
\left[\hat{A}^{\mu(+)}(\mathbf{r}, t), \frac{\partial}{\partial t} \hat{A}^{\nu(-)}(\mathbf{r}', t) \right] &= -\frac{i\hbar}{2\epsilon_0} g^{\mu\nu} \int_{-\infty}^{\infty} e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r}')} \frac{d^3 q}{(2\pi)^3} \\
&= -\frac{i\hbar}{2\epsilon_0} g^{\mu\nu} \delta(\mathbf{r} - \mathbf{r}').
\end{aligned} \tag{29.185}$$

By subtraction of the Hermitian conjugate commutator, and use of (29.182), we are led to the following canonical equal-time commutation relations:

$$[\hat{A}^\mu(\mathbf{r}, t), \hat{\Pi}^\nu(\mathbf{r}', t)] = i\hbar g^{\mu\nu} \delta(\mathbf{r} - \mathbf{r}'). \tag{29.186}$$

29.5.3 The Feynman Photon Propagator

In Sect. 24.1 we introduced the massive Feynman scalar propagator by the definition in (24.4). The definition involves the function $\Delta^+(x)$, and its complex conjugate $\Delta^-(x)$. Since the massless version of $\Delta^+(x)$ also appears in the commutator between $\hat{A}^{\mu(+)}(x)$ and $\hat{A}^{\nu(-)}(x')$ (see (29.178)), one might expect that there exists a close connection between the massless Feynman scalar propagator and some simple bilinear form of the four-potential. To throw light on this matter we consider the mean value of the commutator in (29.178) in the photon vacuum. Since the vacuum state for all $\mathbf{q}$ satisfies (29.99), and the associated bra relation $\langle 0 | \hat{a}_r^\dagger(\mathbf{q}) = 0$, it is obvious that

$$\begin{aligned}
\langle 0 | [\hat{A}^{\mu(+)}(x), \hat{A}^{\nu(-)}(x')] | 0 \rangle &= \langle 0 | \hat{A}^{\mu(+)}(x) \hat{A}^{\nu(-)}(x') | 0 \rangle \\
&= \langle 0 | \hat{A}^\mu(x) \hat{A}^\nu(x') | 0 \rangle.
\end{aligned} \tag{29.187}$$

Thus, we have

$$\langle 0 | \hat{A}^\mu(x) \hat{A}^\nu(x') | 0 \rangle = \frac{i\hbar}{\epsilon_0 c_0^2} (-g^{\mu\nu}) \Delta^+(x - x'). \tag{29.188}$$

The first term in the Feynman propagator in (24.4) also contains the step function $\theta(\tau)$, but (29.189) is correct independent of the time order appearing in $\hat{A}^\mu(x)$ and $\hat{A}^\nu(x')$.

To incorporate the step function in the description we define the time-ordered or T -product by

$$T \left\{ \hat{A}^\mu(x) \hat{A}^\nu(x') \right\} = \begin{cases} \hat{A}^\mu(x) \hat{A}^\nu(x') & t > t' \\ \hat{A}^\nu(x') \hat{A}^\mu(x) & t < t' \end{cases} \quad (29.189)$$

remembering that $t = x^0/c_0$ and $t' = (x')^0/c_0$. In a T -product, the operators are written in chronological order with time running from right to left. The “earlier” operator thus acts “first” on a given ket. With the help of the step function, the T -product can be written

$$T \left\{ \hat{A}^\mu(x) \hat{A}^\nu(x') \right\} = \theta(t - t') \hat{A}^\mu(x) \hat{A}^\nu(x') + \theta(t' - t) \hat{A}^\nu(x') \hat{A}^\mu(x). \quad (29.190)$$

The form in (29.190) together with the result in (29.188), show that the vacuum mean value of the time-ordered product is given by

$$\begin{aligned} \langle 0 | T \left\{ \hat{A}^\mu(x) \hat{A}^\nu(x') \right\} | 0 \rangle &= \frac{i\hbar}{\epsilon_0 c_0^2} \left[\theta(t - t') (-g^{\mu\nu}) \Delta^+(x - x') \right. \\ &\quad \left. + \theta(t' - t) (-g^{\nu\mu}) \Delta^+(x' - x) \right]. \end{aligned} \quad (29.191)$$

Since

$$\Delta^+(-x) = -\Delta^-(x), \quad (29.192)$$

as the reader may verify, and $g^{\nu\mu} = g^{\mu\nu}$, we finally obtain

$$\langle 0 | T \left\{ \hat{A}^\mu(x) \hat{A}^\nu(x') \right\} | 0 \rangle = \frac{i\hbar}{\epsilon_0 c_0^2} G_F^{\mu\nu}(x - x'), \quad (29.193)$$

where

$$G_F^{\mu\nu}(x) = -g^{\mu\nu} \lim_{m \rightarrow 0} \Delta_F(x). \quad (29.194)$$

The mean value on the left side of (29.193) is known as the Feynman photon propagator [155]; see also [373]. Loosely speaking, one may say that the Feynman propagator represents a kind of photon exchange between the space-time points x' and x . Since the expression for the four-potential operator (29.144) contains a summation over polarization modes we in general expect an exchange of four kind of photons: Two transverse photons, and longitudinal and scalar photons (or equivalently gauge and near-field photons). For $t' > t$, photon creation takes place at x' first and thereafter photon annihilation appears at x . For $t < t'$, photon creation at x is followed later on by annihilation at x' . The interpretation of (29.193) in terms of photon exchange will be discussed in some detail in Chap. 30, and we will there see how the covariant formalism puts the exchange of virtual photons in near-field electrodynamics in perspective.

Chapter 30

Matter-Attached Quantized Fields

In this last chapter, we turn our attention towards the picture the covariant formulation offers us of the quantized field–matter interaction in the nonrelativistic regime. In the context of near-field electrodynamics, the always matter-attached longitudinal and scalar photons play a prominent role, and therefore, these photons are in focus in what follows. Although the limitation to nonrelativistic mechanics reduces the field–matter interaction problem considerably, it is in general still a formidable task to determine the temporal evolution of the coupled system when account must be taken of the reaction of the field radiation on the particle dynamics.

We begin our study with an analysis of the covariant photon propagator introduced in Sect. 29.5.3. In four-momentum space the physical interpretation of the propagator becomes clear when the specific choice of Sect. 29.2.1 is made for the polarization vectors. The instantaneous Coulomb interaction now appears by a combination of the scalar photon propagator with a part of the longitudinal photon propagator. The remaining part of the L-propagator has the character of a gauge term of no physical importance. We also show how one can filter out the near-field and gauge photon contributions from the covariant photon propagator.

After having rewritten the standard interaction Lagrangian density in covariant form, we obtain from the Lagrange equations for the electromagnetic field the covariant Maxwell–Lorentz equations for the components of the four-potential. The solution of the four-dimensional wave equation then is expressed in terms of the well-known advanced and retarded scalar Green functions. In scattering experiments, the difference between these Green functions appears. The difference, often called the scattering propagator, is shown to be closely related to the massless Jordan-Pauli propagator.

In Sect. 30.3, we study the perhaps simplest kind of electromagnetic interaction, viz., that between two fixed point charges. In the covariant-formulation of QED this interaction appears as being due to an exchange of scalar photons between the charges. The particle–particle interaction mediated by the scalar photons gives rise to an energy shift of the ground state of the field, and this shift is precisely the Coulomb energy of the two charges. We also discuss how the Coulomb interaction can be described in terms of either near-field or gauge photon exchange.

In the last part of the chapter we turn our attention towards the covariant description of evanescent fields. From a qualitative point of view most of the physics can

be captured via a study of sheet sources. The simplest situation occurs when the current density of the sheet can be assumed to be prescribed. We start in the classical regime with a calculation and a discussion of the longitudinal and scalar parts of the four-potential. We thereafter treat the quantum-field radiation by a prescribed source current without quantum fluctuations. From the Heisenberg equation of motion for the various mode annihilation operators we show that the radiated covariant field is quasi-classical. The chapter is finished with a description of the coherent scalar and longitudinal photon radiation from a sheet source.

30.1 Analysis of the Covariant Photon Propagator

30.1.1 Combined Exchange of Longitudinal and Scalar Photons

In Sect. 24.4.2, it was shown that the Feynman scalar propagator (meson propagator) can be given in the form of a contour integral along a certain contour C_F ; see (24.60). In view of this, it appears that the covariant photon propagator (29.194) has the integral representation

$$G_F^{\mu\nu}(x) = \int_{C_F} G_F^{\mu\nu}(q) e^{-iq_\mu x^\mu} \frac{d^4 q}{(2\pi)^4}, \quad (30.1)$$

where

$$G_F^{\mu\nu}(q) = \frac{-c_0 g^{\mu\nu}}{q_\mu q^\mu + i\epsilon} \quad (30.2)$$

is the wave-vector ($\sim$ momentum) space propagator. The physical role of the transverse, longitudinal and scalar photons in $G_F^{\mu\nu}(q)$ comes to light when the metric tensor elements $g^{\mu\nu}$ are expressed in terms of four linearly independent polarization vectors (29.42).

The interpretation becomes clear when we make the particular choice given in (29.43) and (29.44) for the polarization vectors. In the given frame of reference, the contribution to the momentum space propagator from the transverse photons is given by

$${}_T G_F^{\mu\nu}(q) = \frac{c_0}{q_\mu q^\mu + i\epsilon} \sum_{r=1}^2 \epsilon_r^\mu(q) \epsilon_r^\nu(q). \quad (30.3)$$

Since (29.44) implies that ${}_T G_F^{\mu\nu}$ is zero unless $\mu, \nu = 1, 2, 3$, the nonvanishing part of $\{{}_T G_F^{\mu\nu}\}$ can be written in three-vector notation [$i, j = 1, 2, 3$]. In standard notation one has $q_\mu q^\mu = q_0^2 - \mathbf{q} \cdot \mathbf{q}$, and with the help of (15.52) we obtain

$${}_T G_F^{ij}(q) = \frac{c_0 (\delta_{ij} - \kappa_i \kappa_j)}{q_0^2 - \mathbf{q} \cdot \mathbf{q}} \quad (30.4)$$

with $i\epsilon$ left out. A comparison to the integrand in (14.66) then shows that the propagator in (30.4), apart from a factor $-c_0$, is just our old transverse $\mathbf{q}$ -space propagator, i.e.,

$${}_T G_F^{ij}(\mathbf{q}) = -c_0 G_T^{ij}(\mathbf{q}, \omega). \quad (30.5)$$

The contribution to the momentum space propagator from the longitudinal photon, viz.,

$${}_L G_F^{\mu\nu}(\mathbf{q}) = \frac{c_0}{q_\mu q^\mu + i\epsilon} \epsilon_3^\mu(\mathbf{q}) \epsilon_3^\nu(\mathbf{q}), \quad (30.6)$$

of course also vanishes unless $\mu, \nu = 1, 2, 3$. Reduced to three-vector notation one has

$${}_L G_F^{ij}(\mathbf{q}) = \frac{c_0 \kappa_i \kappa_j}{q_0^2 - \mathbf{q} \cdot \mathbf{q}}. \quad (30.7)$$

The Feynman propagator in (30.7) does not deviate from our old longitudinal Green function $G_L^{ij}(\mathbf{q}, \omega)$ by merely a trivial factor. From the last term in (4.28) one obtains

$$G_L^{ij}(\mathbf{q}, \omega) = -\frac{\kappa_i \kappa_j}{q_0^2}. \quad (30.8)$$

The essential difference between (30.7) and (30.8) originates in the fact that the longitudinal part of the Feynman photon propagator relates to a retarded (with speed c_0) particle–particle interaction, whereas the old Green function describes the longitudinal interaction as instantaneous. The difference between these two points of view stems from the gauge choices (Lorenz and Coulomb), and has no physical (observational) consequences.

The instantaneous Coulomb interaction cannot be obtained from ${}_L G_F^{\mu\nu}$ alone. Thus, one must combine a part of the longitudinal propagator with the scalar photon propagator

$$\begin{aligned} {}_S G_F^{\mu\nu}(\mathbf{q}) &= -\frac{c_0}{q_\mu q^\mu + i\epsilon} \epsilon_0^\mu(\mathbf{q}) \epsilon_0^\nu(\mathbf{q}) \\ &= -\frac{c_0 \eta^\mu \eta^\nu}{q_\mu q^\mu + i\epsilon} = -\frac{c_0 \delta_{\mu 0} \delta_{\nu 0}}{q_\mu q^\mu + i\epsilon}, \end{aligned} \quad (30.9)$$

as we soon shall see. The elements of the momentum space Feynman photon propagator are given by the sum

$$G_F^{\mu\nu}(\mathbf{q}) = {}_T G_F^{\mu\nu}(\mathbf{q}) + {}_L G_F^{\mu\nu}(\mathbf{q}) + {}_S G_F^{\mu\nu}(\mathbf{q}). \quad (30.10)$$

To find out how the instantaneous Coulomb interaction is hidden in the sum of the L and S contributions to $G_F^{\mu\nu}(x)$ (30.1), it is useful to write the unit polarization vector for the longitudinal mode in the *formally covariant* form

$$\{\epsilon_3^\mu\} \equiv \{\kappa^\mu\} = \frac{\{q^\mu\} - (q\eta)\{\eta^\mu\}}{[(q\eta)^2 - q^2]^{1/2}}, \quad (30.11)$$

with the abbreviations (and reference to old notation)

$$q\eta \equiv q_\nu \eta^\mu = q_0, \quad (30.12)$$

$$q^2 \equiv q_\nu q^\nu = q_0^2 - \mathbf{q} \cdot \mathbf{q}. \quad (30.13)$$

I have used the words *formally covariant* for the expression in (30.11) because the quantity $\{\eta^\mu\}$ usually is treated as a space-time independent vector, referring to a particular Lorentz frame. If $\{\eta^\mu\}$ did transform according to the Lorentz transformation it would have to be a function of x . Using (30.11) one may write the longitudinal photon propagator elements given in (30.6) in the form

$${}_L G_F^{\mu\nu}(q) = \frac{c_0}{q^2 + i\epsilon} \frac{[q^\mu - (q\eta)\eta^\mu][q^\nu - (q\eta)\eta^\nu]}{(q\eta)^2 - q^2}. \quad (30.14)$$

For later combination with the scalar photon propagator, we divide the expression in (30.14) as follows:

$${}_L G_F^{\mu\nu}(q) = {}_G G_F^{\mu\nu}(q) + \frac{c_0}{q^2 + i\epsilon} \frac{(q\eta)^2 \eta^\mu \eta^\nu}{(q\eta)^2 - q^2}, \quad (30.15)$$

where

$${}_G G_F^{\mu\nu}(q) = \frac{c_0}{q^2 + i\epsilon} \frac{q^\mu q^\nu - (q\eta)(\eta^\mu q^\nu + q^\mu \eta^\nu)}{(q\eta)^2 - q^2}. \quad (30.16)$$

Since, as announced earlier, we want to add part of ${}_L G_F^{\mu\nu}(q)$ to ${}_S G_F^{\mu\nu}(q)$, it is perhaps not a surprise for the reader in view of the second member on the right side of (30.9) that the term proportional to $\eta^\mu \eta^\nu$ was separated from ${}_L G_F^{\mu\nu}(q)$. It is possible to demonstrate directly that the term ${}_G G_F^{\mu\nu}(q)$ in (30.16) has the character of a gauge term (as indicated by the index G), and therefore it is of no physical importance. Indirectly, this is obvious from the fact that the complete electromagnetic interaction between charged particles is accounted for via the transverse radiation field and the Coulomb field. A straightforward calculation now leads to the result

$${}_L G_F^{\mu\nu}(q) + {}_S G_F^{\mu\nu}(q) = {}_C G_F^{\mu\nu}(q) + {}_G G_F^{\mu\nu}(q), \quad (30.17)$$

where

$${}_C G_F^{\mu\nu}(q) = \frac{c_0 \eta^\mu \eta^\nu}{(q\eta)^2 - q^2} = \frac{c_0 \delta_{\mu 0} \delta_{\nu 0}}{\mathbf{q} \cdot \mathbf{q}}. \quad (30.18)$$

During the derivation of the expression in (30.18) a factor $q^2/(q^2 + i\epsilon)$ appears. Since the infinitesimal quantity $i\epsilon$ only is of importance when the relevant expression has a pole, as indicated earlier, the factor above can be set to 1. The “propagator” in (30.18) has been given a subscript C , because it relates to the instantaneous Coulomb interaction between charges. In order to prove this we consider its configuration space representative, viz.,

$${}_cG_F^{\mu\nu}(x) = \int_{-\infty}^{\infty} {}_cG_F^{\mu\nu}(q) e^{iq_\mu x^\mu} \frac{d^4q}{(2\pi)^4}. \quad (30.19)$$

By inserting (29.39) and (30.18) into (30.19) one obtains

$${}_cG_F^{\mu\nu}(x) = c_0 \delta_{\mu 0} \delta_{\nu 0} \int_{-\infty}^{\infty} e^{-ic_0 q_0 t} \frac{dq_0}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\mathbf{q} \cdot \mathbf{r}}}{\mathbf{q} \cdot \mathbf{q}} \frac{d^3q}{(2\pi)^3}. \quad (30.20)$$

The integral over q_0 is a delta function, and the integral over $\mathbf{q}$ -space is given in (9.62). Thus,

$${}_cG_F^{\mu\nu}(x) = \frac{c_0}{4\pi r} \delta(c_0 t) g^{\mu 0} g^{\nu 0}. \quad (30.21)$$

Now, we see that the propagator ${}_cG_F^{\mu\nu}(x)$ has a time dependence $\delta(c_0 t)$ and a space dependence r^{-1} , i.e., the characteristics of an instantaneous Coulomb interaction; cf. (9.64).

30.1.2 Near-Field and Gauge Photon Exchange

In the preceding subsection we obtained the contributions of the longitudinal and scalar photons to the Feynman propagator by a polarization vector analysis of the metric tensor, $g^{\mu\nu}$. Now, we shall indicate how the roles of the near-field and gauge photons in the covariant propagator may be determined.

The connection between the longitudinal and scalar modes and the near-field and gauge modes is given by (29.55) for the specific choice in (29.43) and (29.44). The related plane-wave expansions of the positive-frequency parts of the classical gauge and near-field four-component potentials are given in (29.56) and (29.57). The orthogonal real and imaginary polarization unit vectors for the gauge and near-field modes thus are

$$\{G^\mu\} = \frac{1}{\sqrt{2}}(1, \kappa), \quad (30.22)$$

and

$$\{N^\mu\} = \frac{i}{\sqrt{2}}(1, -\kappa), \quad (30.23)$$

respectively. Since, as the reader may show,

$$G^\mu G^\nu - N^\mu N^\nu = \delta_{\mu 0} \delta_{\nu 0} + (1 - \delta_{\mu 0})(1 - \delta_{\nu 0}) \kappa^\mu \kappa^\nu, \quad (30.24)$$

and

$$\sum_{r=1}^2 \epsilon_r^\mu \epsilon_r^\nu = (1 - \delta_{\mu 0})(1 - \delta_{\nu 0})(\delta_{\mu\nu} - \kappa^\mu \kappa^\nu), \quad (30.25)$$

where $\{\kappa^\mu\} = (0, \kappa)$, the Kronecker delta has the expansion

$$\delta_{\mu\nu} = \sum_{r=1}^2 \epsilon_r^\mu \epsilon_r^\nu + G^\mu G^\nu - N^\mu N^\nu. \quad (30.26)$$

We have seen in Sect. 29.4.3 that the Hamilton operator belonging to the gauge and near-field modes takes the standard form (29.167) in the indefinite metric formalism provided the metric M is chosen in such a manner that (29.149) and (29.150) are satisfied. In this metric the commutator between $A^{\mu(+)}(x)$ and $\bar{A}^{v(+)}(x')$ is given by

$$\left[A^{\mu(+)}(x), \bar{A}^{v(+)}(x') \right] = \frac{i\hbar}{\epsilon_0 c_0^2} (-g^{\mu\nu}) \Delta^+(x - x'), \quad (30.27)$$

cf. (29.178). In view of the relations in (29.149) and (29.150), one hence obtains

$$\left[A^{\mu(+)}(x), A^{v(-)}(x') \right] = \frac{i\hbar}{\epsilon_0 c_0^2} \delta_{\mu\nu} \Delta^+(x - x'). \quad (30.28)$$

As in Sect. 29.4, the operator symbol $\wedge$ has been omitted in the equations above. The steps leading from the commutator in (30.27) (or in (30.28)) to the Feynman photon propagator can be taken in the same manner as in Sect. 29.5.3. Thus, one obtains for the vacuum mean value of the time-ordered product

$$\subset 0|T\{A^\mu(x)A^v(x')\}|0 \supset = \langle 0|MT\{A^\mu(x)A^v(x')\}|0 \rangle = \frac{i\hbar}{\epsilon_0 c_0^2} \mathcal{G}^{\mu\nu}(x - x'), \quad (30.29)$$

where

$$\mathcal{G}^{\mu\nu}(x) = \delta_{\mu\nu} \lim_{m \rightarrow 0} \Delta_F(x). \quad (30.30)$$

The first member of (30.29) follows by utilizing (29.135). The propagator in (30.30) has, like the Feynman photon propagator, $G_F^{\mu\nu}(x)$, a contour integral representation

$$\mathcal{G}^{\mu\nu}(x) = \int_{C_F} \mathcal{G}^{\mu\nu}(q) e^{-iq_\mu x^\mu} \frac{d^4 q}{(2\pi)^4}, \quad (30.31)$$

where

$$\mathcal{G}^{\mu\nu}(q) = \frac{c_0 \delta_{\mu\nu}}{q_\mu q^\mu + i\epsilon}. \quad (30.32)$$

The expansion of the Kronecker delta (30.26) enables one to filter out from the momentum space propagator the near-field and gauge photon contributions, viz.,

$$_{\text{NF}}\mathcal{G}^{\mu\nu}(q) = \frac{-c_0}{q_\mu q^\mu + i\epsilon} N^\mu(q) N^\nu(q), \quad (30.33)$$

and

$$_G\mathcal{G}^{\mu\nu}(q) = \frac{c_0}{q_\mu q^\mu + i\epsilon} G^\mu(q) G^\nu(q). \quad (30.34)$$

The various components of the symmetric G and NF momentum space propagators are either equal or of opposite sign. Thus,

$$_{\text{NF}}\mathcal{G}^{00}(q) = {}_G\mathcal{G}^{00}(q), \quad (30.35)$$

$${}_{\text{NF}}\mathcal{G}^{ij}(q) = {}_G\mathcal{G}^{ij}(q), \quad (30.36)$$

and

$${}_{\text{NF}}\mathcal{G}^{i0}(q) = -{}_G\mathcal{G}^{0i}(q), \quad (30.37)$$

where $i, j = 1, 2, 3$. In configuration space only the diagonal elements of the gauge and near-field photon propagators are different from zero.

30.2 Field–Particle Interaction in Covariant Notation

30.2.1 Interaction Lagrangian Density and Wave Equation

To describe the interaction between the electromagnetic field and the particles let us consider the interaction Lagrangian density given in (25.37). In covariant gauges, where the potentials ϕ/c_0 and $\mathbf{A}$ form a four-vector, the interaction Lagrangian density $\mathcal{L}_1^{\text{ST}} \equiv \mathcal{L}_1$ can be written in the covariant form

$$\mathcal{L}_1(x) = -j_\mu(x)A^\mu(x), \quad (30.38)$$

as the reader may verify by taking the scalar product of the covariant current density four-vector (29.6) and the contravariant four-vector potential (29.5). From the Lagrange equations for the fields, namely,

$$\sum_{\nu=0}^3 \partial_\nu \left(\frac{\partial(\mathcal{L}_F + \mathcal{L}_1)}{\partial(\partial_\nu A_\mu)} \right) - \frac{\partial}{\partial A_\mu} (\mathcal{L}_F + \mathcal{L}_1) = 0, \quad (30.39)$$

we are led to the inhomogeneous wave equations for the components of the four-vector potential. The equations of motion for the particles in the presence of the potential $\{A^\mu\}$ can be obtained from the Lagrange formalism adding a suitable particle Lagrangian density to $\mathcal{L}_F + \mathcal{L}_1$. For what follows such an extension is not necessary. By writing the interaction Lagrangian density in the form $\mathcal{L}_1 = -j^\mu A_\mu$, we immediately get

$$\frac{\partial \mathcal{L}_1}{\partial A_\mu} = -j^\mu. \quad (30.40)$$

Since $\mathcal{L}_1$ does not depend on the derivatives of the potential, $\partial_\nu A_\mu$, the term in (30.40) is the only correction to the Lagrange equation for the μ -component of the free field. Utilizing (29.30), (29.31) and (30.40), one obtains the following four-dimensional wave equation for the potential:

$$\epsilon_0 c_0^2 \partial_\nu \partial^\nu A^\mu(x) = j^\mu(x). \quad (30.41)$$

When written in the form

$$\square A^\mu(x) = -\mu_0 j^\mu(x), \quad (30.42)$$

the four-dimensional wave equation in a manifest manner can be identified with (2.14) and (2.15). We emphasize that (30.42) presupposes that the potentials satisfy the Lorenz condition (29.32), or just a slightly generalized condition (see below).

Returning to the standard approach, presented in Sects. 29.1.2 and 29.1.3, it is obvious that the inhomogeneous Maxwell–Lorentz equations written in terms of the potentials become

$$\square A^\mu(x) + \partial^\mu(\partial_\nu A^\nu(x)) = -\mu_o j^\mu(x). \quad (30.43)$$

As we already know, these equations are invariant under the gauge transformation

$$A^\mu(x) \Rightarrow A'^\mu(x) = A^\mu(x) - \partial^\mu \chi(x). \quad (30.44)$$

The gauge transformation in (30.44) is covariant. A covariant gauge, defined to satisfy the condition

$$\partial_\mu A^\mu = K, \quad (30.45)$$

where K is a constant, loses its covariance when a noncovariant condition is imposed on the gauge function $\chi(x)$. For a covariant gauge, e.g., the Lorenz gauge ($K = 0$), (30.43) is reduced to (30.42).

Under a gauge transformation the density of the interaction Lagrangian changes as follows:

$$\mathcal{L}_I \Rightarrow \mathcal{L}'_I = \mathcal{L}_I + j_\mu(x) \partial^\mu \chi(x). \quad (30.46)$$

By means of the equation of continuity (2.108), which in covariant notation reads

$$\partial_\mu j^\mu(x) = 0, \quad (30.47)$$

the last term in (30.46) equals

$$j_\mu(x) \partial^\mu \chi(x) = \partial^\mu (j_\mu(x) \chi(x)). \quad (30.48)$$

Although the Lagrangian density thus is not invariant, the addition of a four-divergence to $\mathcal{L}_I$ does not alter the field equations. This is so because the standard space–time action integrals of $\mathcal{L}_I$ and $\mathcal{L}'_I$ are identical. To prove this one uses Gauss' divergence theorem in four dimensions on the four-divergence.

30.2.2 Retarded and Advanced Propagators: In- and Out-States

In order to accomplish the solution of the four-dimensional wave equation in (30.42) in terms of a Green function formalism we first solve the auxiliary problem

$$\square D(x - x') = -\delta^{(4)}(x - x') \quad (30.49)$$

for the Green function $D(x - x')$. The quantity

$$\delta^{(4)}(x - x') = \delta(x_0 - x'_0)\delta(\mathbf{r} - \mathbf{r}') \quad (30.50)$$

is the four-dimensional delta function, and the d'Alembertian operator in (30.49) acts on the x -coordinates of the Green function, i.e., $\square = \square_x$.

Let us assume that there exists an integral representation for $D(x)$ that is

$$D(x) = \int_{-\infty}^{\infty} D(q) e^{-iqx} \frac{d^4 q}{(2\pi)^4}. \quad (30.51)$$

By inserting this, together with the Fourier integral expansion of the delta function

$$\delta^{(4)}(x) = \int_{-\infty}^{\infty} e^{-iqx} \frac{d^4 q}{(2\pi)^4}, \quad (30.52)$$

into (30.49) one obtains a q -space Green function

$$D(q) = -q^{-2} = -(q_\mu q^\mu)^{-1}. \quad (30.53)$$

This expression for $D(q)$ shows that the integrand in (30.51) is singular, and the integral expression for $D(x)$ thus ambiguous. To give a definite meaning to the integral we consider q^0 as a complex variable, and treat the integral as a contour integral in the q^0 -plane. Thus,

$$D(x) = - \int_C \frac{e^{-iq_\mu x^\mu}}{q_\mu q^\mu} \frac{d^4 q}{(2\pi)^4} \quad (30.54)$$

where C indicates the contour in the q^0 -plane. A comparison to (24.56) tells us that $c_0 D(x)$ is identical to $\Delta(x)$ for a massless particle, that is

$$D(x) = \frac{1}{c_0} \Delta(x; Q_C \rightarrow 0). \quad (30.55)$$

We now choose a contour that encloses both poles on the real q^0 -axis (located at $q^0 = \pm |q|$). We know from the analysis in Sect. 24.4.1 that Δ equals the Jordan-Pauli propagator if the contour ($C = C_{JP}$) is circulated counter-clockwise. Here, we use this circulation *only* for $x^0 = c_0 \tau < 0$. The explicit expression for the Jordan-Pauli propagator, given in (24.10), then shows that only the first delta function, $\delta[(R/c_0) + \tau]$ contributes to the Δ in (30.55). With the counter-clockwise contour circulation around both poles for $x^0 < 0$, we obtain in standard notation the Green function

$$D_A(r, t) = \theta(-c_0 t) \frac{\delta(r + c_0 t)}{4\pi t}. \quad (30.56)$$

The subscript A indicates that D_A is the so-called *advanced* Green function. The name stems from the fact that the source-point time is later than the observation-point time; see below. For $x^0 > 0$, we circulate the poles clockwise. This means that the result in (24.10) must be multiplied by minus one, and now only the delta

function $\delta[(R/c_0) - \tau]$ contributes. In standard notation we thus end up with the *retarded* Green function

$$D_R(\mathbf{r}, t) = \theta(c_0 t) \frac{\delta(r - c_0 t)}{4\pi r}. \quad (30.57)$$

This Green function relates to a situation where the source-point time is earlier than the observation-point time; see below.

It is apparent from the analysis in Sect. 14.6 that the two Green functions (propagators) above can be written in covariant notation as follows:

$$D_R(x) = \frac{1}{2\pi} \theta(x^0) \delta(x^2), \quad (30.58)$$

$$D_A(x) = \frac{1}{2\pi} \theta(-x^0) \delta(x^2). \quad (30.59)$$

On the basis of these propagators two important types of solutions to the wave equation in (30.42) are obtained, viz.,

$$A^\mu(x) = A_{\text{inc}}^\mu(x) + \mu_0 \int_{-\infty}^{\infty} D_R(x - x') j^\mu(x') d^4 x', \quad (30.60)$$

and

$$A^\mu(x) = A_{\text{out}}^\mu(x) + \mu_0 \int_{-\infty}^{\infty} D_A(x - x') j^\mu(x') d^4 x'. \quad (30.61)$$

Let us first consider the interpretation of (30.60). Since the current density necessarily is localized in time (and space), and the retarded Green function is zero for $x_0 < x'_0$, the integral vanishes for $x_0 \rightarrow -\infty$. The potential $A_{\text{inc}}^\mu(x)$, which is a solution to the homogeneous wave equation, hence can be interpreted as the “incident” (or “incoming”) potential (specified at $x_0 \rightarrow -\infty$). Let us next consider the interpretation of (30.61). The presence of the advanced Green function implies that the integral vanishes for $x_0 \rightarrow \infty$. The solution A_{out}^μ to the homogeneous wave equation therefore represents the “outgoing” potential (specified at $x_0 \rightarrow \infty$).

A *given* physical scattering experiment may be characterized *either* by (30.60) or by (30.61), but the potential $A^\mu(x)$ on the left side of these equations must be the same. The difference between the outgoing and incoming fields, i.e.,

$$A_{\text{scatt}}^\mu(x) = A_{\text{out}}^\mu(x) - A_{\text{inc}}^\mu, \quad (30.62)$$

thus represents what might be called the “scattered” field. The scattered field is given by

$$A_{\text{scatt}}^\mu(x) = \mu_0 \int_{-\infty}^{\infty} D_{\text{scatt}}(x - x') j^\mu(x') d^4 x', \quad (30.63)$$

and relates to the current density via a scattering propagator D_{scatt} which is the difference between D_R and D_A :

$$D_{\text{scatt}}(x - x') = D_R(x - x') - D_A(x - x'). \quad (30.64)$$

The scattering propagator and the massless Jordan–Pauli propagator are closely related. In standard notation one thus has

$$c_0 D_{\text{scatt}}(R, \tau) = -\Delta_{\text{JP}}(R, \tau; Q_C \rightarrow 0). \quad (30.65)$$

30.3 Interaction Between Two Fixed Charges: Exchange of Scalar Photons

30.3.1 Prescribed Particle Dynamics: Hamiltonian for Field Evolution

To describe the dynamics of a coupled field–particle system, e.g., the dynamics of the coupled Dirac and Maxwell fields, on the basis of a Lagrangian formalism one needs, as we have seen, the Lagrangian densities of the particles, fields, and the interaction. In cases where the particle dynamics is prescribed one only needs to study the time evolution of the field. For such purposes it is sufficient to know the Lagrangian densities of the field ($\mathcal{L}_F$) and the field–particle interaction ($\mathcal{L}_I$). In the covariant theory a suitable choice for $\mathcal{L}_F$ was given in (29.26), and the expression for $\mathcal{L}_I$ is that in (30.38). The associated density $\mathcal{H}_F(x)$ of the field Hamiltonian is given in (29.71), and the density of the interaction Hamiltonian, which is just $\mathcal{H}_I(x) = -\mathcal{L}_I(x)$, thus becomes

$$\mathcal{H}_I(x) = j_\mu(x) A^\mu(x). \quad (30.66)$$

The Hamilton operator needed to describe the evolution of the field in the presence of a prescribed (external) covariant current density $\{j_\mu^{\text{ext}}\}$ hence takes the form

$$H = \sum_{\mathbf{q}, r} \hbar \omega_{\mathbf{q}} \left(-\zeta_r \bar{a}_r(\mathbf{q}) a_r(\mathbf{q}) + \frac{1}{2} \right) + \int_{-\infty}^{\infty} j_\mu^{\text{ext}}(x) A^\mu(x) d^3r, \quad (30.67)$$

where for discrete mode quantization

$$A^\mu(x) = L^{-3/2} \sum_{\mathbf{q}, r} \left(\frac{\hbar}{2\epsilon_0 \omega_{\mathbf{q}}} \right)^{1/2} \epsilon_r^\mu(\mathbf{q}) \left(a_r(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{r}} + \bar{a}_r(\mathbf{q}) e^{-i\mathbf{q} \cdot \mathbf{r}} \right). \quad (30.68)$$

The expression in (30.67) relates to covariant quantization with an indefinite metric, as described in Sect. 29.4, and as there, the operator symbol ($\wedge$) is omitted in the notation. The annihilation ($a_r(\mathbf{q})$) and creation ($\bar{a}_r(\mathbf{q})$) operators depend on time in general. The first part of (30.67) is the free-field Hamilton operator of the transverse, longitudinal, and scalar photon modes, and of the vacuum.

Let us now consider the particularly simple example where the quantized field is coupled to two fixed point charges q_1 and q_2 located at the space points $\mathbf{r}_1$ and $\mathbf{r}_2$. In the rest frame of the charges the four-current density is given by $\{j_\mu^{\text{ext}}(x)\} = (c_0\rho, \mathbf{0})$, where

$$\rho(\mathbf{r}) = q_1\delta(\mathbf{r} - \mathbf{r}_1) + q_2\delta(\mathbf{r} - \mathbf{r}_2) \quad (30.69)$$

is the spatial charge density. For brevity, the reference “ext” is omitted from $\rho(\mathbf{r})$. In the chosen inertial system the field–particle interaction only involves scalar photons (via $A^0(x)$) because just the first component of $\{j_\mu^{\text{ext}}\}$ is nonvanishing. The interaction Hamiltonian in consequence is given by

$$\begin{aligned} H_1 &= \int_{-\infty}^{\infty} c_0\rho(\mathbf{r})A^0(\mathbf{r})d^3r \\ &= c_0q_1A^0(\mathbf{r}_1) + c_0q_2A^0(\mathbf{r}_2), \end{aligned} \quad (30.70)$$

where, in view of (29.43) and (29.44), the mode expansion for A^0 becomes

$$A^0(\mathbf{r}) = \sum_q \left(\frac{\hbar}{2\epsilon_0\omega_q L^3} \right)^{1/2} (a_0(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}} + \bar{a}_0(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{r}}). \quad (30.71)$$

For what follows it is convenient to write the interaction Hamiltonian in the form

$$H_1 = \sum_q \hbar\omega_q (\Delta^*(\mathbf{q})a_0(\mathbf{q}) + \Delta(\mathbf{q})\bar{a}_0(\mathbf{q})), \quad (30.72)$$

where

$$\Delta(\mathbf{q}) = \frac{c_0}{\hbar\omega_q} \left(\frac{\hbar}{2\epsilon_0\omega_q L^3} \right)^{1/2} \rho(\mathbf{q}). \quad (30.73)$$

The quantity

$$\begin{aligned} \rho(\mathbf{q}) &= \int_{-\infty}^{\infty} \rho(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}}d^3r \\ &= q_1e^{-i\mathbf{q}\cdot\mathbf{r}_1} + q_2e^{-i\mathbf{q}\cdot\mathbf{r}_2} \end{aligned} \quad (30.74)$$

is the charge density in reciprocal space.

30.3.2 Energy Shift of the Ground State of the Field

In the absence of matter, we are left with the free-field Hamiltonian (first part of (30.67)). Since we know that the Gupta–Bleuler–Lorenz condition implies that the longitudinal and scalar photons cannot give a net contribution to the mean value of the field energy in free space, all possible energies of the free field are determined by the number of transverse photons. The global ground state of the field is the

photon vacuum, denoted as before by $|0\rangle$. The presence of the two charges modifies the ground state of the field, as we shall realize below. Since only the scalar photon modes participate in the field–matter interaction it is sufficient here to consider the part of the Hamiltonian in (30.67) which relates to the scalar photons, viz.,

$$H_S = \sum_{\mathbf{q}} H_S(\mathbf{q}), \quad (30.75)$$

where

$$H_S(\mathbf{q}) = \hbar\omega_{\mathbf{q}} \left(-\bar{a}_0(\mathbf{q})a_0(\mathbf{q}) + \Delta^*(\mathbf{q})a_0(\mathbf{q}) + \Delta(\mathbf{q})\bar{a}_0(\mathbf{q}) + \frac{1}{2} \right). \quad (30.76)$$

The Hamilton operator in (30.76) can easily be diagonalized by introduction of the new operator

$$b_0(\mathbf{q}) = a_0(\mathbf{q}) - \Delta(\mathbf{q}), \quad (30.77)$$

and its adjoint

$$\bar{b}_0(\mathbf{q}) = \bar{a}_0(\mathbf{q}) - \Delta^*(\mathbf{q}). \quad (30.78)$$

The new operators $b_0(\mathbf{q})$ and $\bar{b}_0(\mathbf{q})$ impose translations on $a_0(\mathbf{q})$ and $\bar{a}_0(\mathbf{q})$, and since

$$[b_0(\mathbf{q}), \bar{b}_0(\mathbf{q}')] = -\delta_{\mathbf{q}\mathbf{q}'}, \quad (30.79)$$

as the reader may realize with the help of (29.146), these operators can be considered as annihilation and creation operators for scalar photons in a new indefinite metric defined here to give $\bar{b}_0(\mathbf{q}) = -b_0^\dagger(\mathbf{q})$. Expressed in terms of the new operators the Hamiltonian in (30.76) takes the form

$$H_S(\mathbf{q}) = \hbar\omega_{\mathbf{q}} \left(-\bar{b}_0(\mathbf{q})b_0(\mathbf{q}) + \Delta(\mathbf{q})\Delta^*(\mathbf{q}) + \frac{1}{2} \right). \quad (30.80)$$

To within a constant $|\Delta(\mathbf{q})|^2$, this is a usual harmonic-oscillator Hamiltonian.

The $\mathbf{q}$ -mode state $|\tilde{0}_{\mathbf{q}}\rangle$, defined by

$$b_0(\mathbf{q})|\tilde{0}_{\mathbf{q}}\rangle = 0, \quad (30.81)$$

obviously is the ground state of $H_S(\mathbf{q})$. The state has an eigenvalue $\hbar\omega_{\mathbf{q}} (|\Delta(\mathbf{q})|^2 + \frac{1}{2})$ which thus is shifted from the vacuum energy $\hbar\omega_{\mathbf{q}}/2$ by an amount $\hbar\omega_{\mathbf{q}}|\Delta(\mathbf{q})|^2$. Use of (30.77) shows that

$$a_0(\mathbf{q})|\tilde{0}_{\mathbf{q}}\rangle = \Delta(\mathbf{q})|\tilde{0}_{\mathbf{q}}\rangle. \quad (30.82)$$

The state $|\tilde{0}_{\mathbf{q}}\rangle$ thus is an eigenstate of the annihilation operator $a_0(\mathbf{q})$. Such a state is a coherent state [345–350], here for the scalar photon mode $\mathbf{q}0$.

The total shift ΔE_0 of the ground state energy of the field is obtained by summing the quantity $\hbar\omega_q |\Delta(\mathbf{q})|^2$ over all scalar modes. Hence,

$$\begin{aligned}\Delta E_0 &= \sum_{\mathbf{q}} \hbar\omega_q |\Delta(\mathbf{q})|^2 \\ &\rightarrow \int_{-\infty}^{\infty} \frac{\rho(\mathbf{q})\rho^*(\mathbf{q})}{2\epsilon_0 q^2} \frac{d^3 q}{(2\pi)^3}.\end{aligned}\quad (30.83)$$

The last expression, which holds in the continuum limit, follows from (30.73) and the rule in (23.1). A comparison to (9.60) shows that ΔE_0 is just the energy of the longitudinal electric field, or equivalently the Coulomb energy

$$\Delta E_0 = \epsilon_{\text{self}}^1 + \epsilon_{\text{self}}^2 + \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (30.84)$$

of the two charges, as we have learned from the analysis in Sect. 9.3.2. The first two terms of (30.84) are the (infinite) self-energies of the two charges, and the last term is the Coulomb interaction energy between them. In the covariant formalism the Coulomb energy thus appears to originate in the fixed charges interaction with the scalar photons.

Let us finally note that all the energy levels of the harmonic oscillator associated with the scalar mode $\mathbf{q}$ are shifted by the same amount, $\hbar\omega_q |\Delta(\mathbf{q})|^2$. To prove this we proceed in the usual manner: Let $N_0 = -\bar{b}_0(\mathbf{q})b_0(\mathbf{q})$ be the scalar photon number operator (cf. (29.101) and (30.80)), and let $N_0|n_0\rangle = n_0|n_0\rangle$ be the associated eigenvalue problem. Using the commutator relation in (30.79) for $\mathbf{q}' = \mathbf{q}$, it is easily shown that

$$N_0(\bar{b}_0|n_0\rangle) = (n_0 + 1)(\bar{b}_0|n_0\rangle). \quad (30.85)$$

From this relation one can conclude that $\bar{b}_0|n_0\rangle$ is an eigenstate for the number operator with an eigenvalue, $n_0 + 1$, which is one larger than that of the state $|n_0\rangle$. The result in (30.85) immediately leads to the equation

$$H_S(\mathbf{q})(\bar{b}_0^n(\mathbf{q})|\tilde{0}_q\rangle) = \hbar\omega_q \left(n + \frac{1}{2} + |\Delta(\mathbf{q})|^2\right) (\bar{b}_0^n(\mathbf{q})|\tilde{0}_q\rangle), \quad (30.86)$$

which shows that $\bar{b}_0^n|\tilde{0}_q\rangle$ is the n th (unnormalized) eigenstate of H_S . This state has an energy which is $n\hbar\omega_q$ higher than that of the new ground state $|\tilde{0}_q\rangle$. Obviously, all oscillator levels are shifted with the same amount $\hbar\omega_q |\Delta(\mathbf{q})|^2$, as claimed above.

30.3.3 Reinterpretation of Coulomb's Law

The exact result obtained for the energy shift of the ground state (30.83) can be reached also by second-order perturbation theory, and obtained in this manner an interesting and simple reinterpretation of the Coulomb interaction occurs. Let $|0\rangle$ be the global ground state of the free field and E_0 the unperturbed energy of this non-degenerate state. To second order in the interaction Hamiltonian H_I of (30.72) the energy shift of the ground state is given by

$$\Delta E_0 = \langle 0|H_I|0\rangle + \sum_n \frac{\langle 0|H_I|\psi_n\rangle\langle\psi_n|H_I|0\rangle}{E_0 - E_n}, \quad (30.87)$$

where the summation is over all excited states, $|\psi_n\rangle$, the unperturbed energies of these states being E_n . Since H_I is linear in the $a_0(\mathbf{q})$ and $\bar{a}_0(\mathbf{q})$ operators, the first term in (30.87) is zero. Furthermore, because these operators can only create or destroy a single scalar photon, only intermediate (excited) states of the type $|1_0(\mathbf{q})\rangle$ can contribute to the second part of (30.87). For intermediate states containing just one scalar photon of energy $\hbar\omega_q$ the energy denominator becomes $E_0 - (E_0 + \hbar\omega_q) = -\hbar\omega_q$. The remarks above thus lead to an energy shift

$$\Delta E_0 = - \sum_q (\hbar\omega_q)^{-1} \langle 0|H_I|1_0(\mathbf{q})\rangle \langle 1_0(\mathbf{q})|H_I|0\rangle. \quad (30.88)$$

The interaction Hamiltonian is Hermitian in the new metric that is

$$H_I = \bar{H}_I, \quad (30.89)$$

as the reader may verify from (30.72). By inserting $\bar{a}_0 = -a_0^\dagger$ (29.149) into this equation it becomes clear that the operator H_I is antihermitian in the usual sense, i.e.,

$$H_I = -H_I^\dagger. \quad (30.90)$$

In consequence of this, one obtains the relation

$$\langle 0|H_I|1_0(\mathbf{q})\rangle = -\langle 1_0(\mathbf{q})|H_I|0\rangle^* \quad (30.91)$$

between the matrix elements in (30.88). According to the well known selection rules for the harmonic oscillator we have

$$\langle 0|a_0(\mathbf{q}')|1_0(\mathbf{q})\rangle = \delta_{\mathbf{q}\mathbf{q}'}, \quad (30.92)$$

and, of course

$$\langle 0|a_0^\dagger(\mathbf{q}')|1_0(\mathbf{q})\rangle = 0. \quad (30.93)$$

Therefore, the following expression for the matrix element on the left side of (30.91) is obtained:

$$\langle 0|H_1|1_0(\mathbf{q})\rangle = \hbar\omega_q \Delta^*(\mathbf{q}). \quad (30.94)$$

By combining (30.88), (30.91) and (30.94) one obtains from the second-order perturbation theory an energy shift

$$\Delta E_0 = \sum_{\mathbf{q}} \hbar\omega_q |\Delta(\mathbf{q})|^2, \quad (30.95)$$

which is identical to the one found by the exact calculation; see (30.83).

The expression in (30.88) indicates that the Coulomb energy may be considered as originating in two-step scalar photon processes. Let us first assume that only the charge q_1 is present. The field, initially in the vacuum state $|0\rangle$, makes a transition to the intermediate state $|1_0(\mathbf{q})\rangle$ by the virtual emission of a scalar photon from q_1 . The photon then is reabsorbed by q_1 and the field returns to the ground state. In this picture the Coulomb self-energy ϵ_{self}^1 in (30.84) thus appears as due to a virtual emission and reabsorption of a scalar photon by q_1 . An analogous picture of course emerges for the self-energy ϵ_{self}^2 of the particle q_2 . The two self-energies are proportional to q_1^2 and q_2^2 , respectively. The Coulomb interaction energy (last term in (30.84)), which is proportional to $q_1 q_2$, appears as stemming from two scalar photon processes: (1) A virtual emission of the photon from q_1 followed by a reabsorption by q_2 and (2) the inverse process, in which q_2 emits and q_1 absorbs. A schematic illustration of these scalar photon processes is shown in Fig. 30.1.

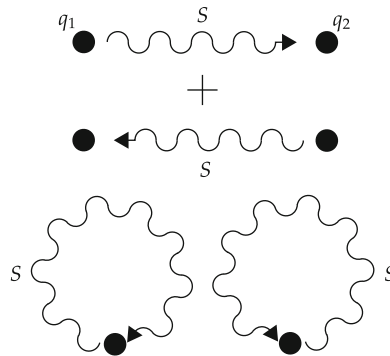


Fig. 30.1 Schematic diagrams illustrating that the Coulomb energy of two *fixed* point charges (q_1 and q_2) in the covariant description of quantum electrodynamics originates in the exchange of scalar photons. The contribution to the Coulomb *interaction energy* from a given field mode ($\mathbf{q}$) is associated with the sum of the two single-photon exchange processes shown in the *upper parts* of the figure. The Coulomb *self-energy* of the particles is associated with a radiative reaction processes where a scalar photon virtually is emitted and then reabsorbed in the given particle, as indicated by the Feynman diagrams in the *bottom* of the figure

30.4 Coulomb Interaction: The Near-Field and Gauge Photon Picture

It is instructive to consider the interaction between two fixed charges as this appears in terms of gauge and near-field photons. In view of the rewriting leading from (30.76) to (30.80) we introduce new annihilation operators for gauge ($\tilde{a}_G$) and near-field ($\tilde{a}_{\text{NF}}$) photons via the definitions

$$\tilde{a}_G(\mathbf{q}) \equiv \frac{1}{\sqrt{2}} (a_L(\mathbf{q}) + b_0(\mathbf{q})), \quad (30.96)$$

$$\tilde{a}_{\text{NF}}(\mathbf{q}) \equiv \frac{i}{\sqrt{2}} (a_L(\mathbf{q}) - b_0(\mathbf{q})). \quad (30.97)$$

The relation in (30.77) between the scalar photon operators $a_0(\mathbf{q})$ and $b_0(\mathbf{q})$ makes the connection between the old ((29.122) and (29.123)) and new ((30.96) and (30.97)) annihilation operators. For quantization with an indefinite metric in Hilbert space the adjoints of $\tilde{a}_G(\mathbf{q})$ and $\tilde{a}_{\text{NF}}(\mathbf{q})$ are

$$\bar{\tilde{a}}_G(\mathbf{q}) = \frac{1}{\sqrt{2}} (\bar{a}_L(\mathbf{q}) + \bar{b}_0(\mathbf{q})), \quad (30.98)$$

$$\bar{\tilde{a}}_{\text{NF}}(\mathbf{q}) = \frac{i}{\sqrt{2}} (-\bar{a}_L(\mathbf{q}) + \bar{b}_0(\mathbf{q})). \quad (30.99)$$

The Hamiltonian which describes the evolution of the longitudinal and scalar parts of the field in the presence of the two charges, viz.,

$$H_L + H_S = \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} [\bar{a}_L(\mathbf{q}) a_L(\mathbf{q}) - \bar{b}_0(\mathbf{q}) b_0(\mathbf{q}) + |\Delta(\mathbf{q})|^2 + 1], \quad (30.100)$$

can be written in terms of the G- and NF-operators inserting the inverse of (30.96)–(30.99) into (30.100). Thus,

$$\begin{aligned} H^{\text{NFG}} &= \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} [i (\bar{\tilde{a}}_{\text{NF}}(\mathbf{q}) \tilde{a}_G(\mathbf{q}) - \bar{\tilde{a}}_G(\mathbf{q}) \tilde{a}_{\text{NF}}(\mathbf{q})) \\ &\quad + |\Delta(\mathbf{q})|^2 + 1]. \end{aligned} \quad (30.101)$$

With a new metric $\tilde{M}$ designed so that

$$\bar{b}_0 = \tilde{M} b_0^\dagger \tilde{M} = -b_0^\dagger, \quad (30.102)$$

and $\bar{a}_L = a_L^\dagger$ as before, one obtains

$$i \bar{\tilde{a}}_{\text{NF}}(\mathbf{q}) = \tilde{a}_G^\dagger(\mathbf{q}), \quad (30.103)$$

$$-i\tilde{a}_G(\mathbf{q}) = \tilde{a}_{\text{NF}}(\mathbf{q}). \quad (30.104)$$

In the new metric the Hamilton operator H^{NFG} takes the form of a sum of harmonic Hamiltonians for the $\mathbf{q}$ -modes of the gauge and near-field variables that is

$$H^{\text{NFG}} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left[\tilde{a}_G^\dagger(\mathbf{q})\tilde{a}_G(\mathbf{q}) + \tilde{a}_{\text{NF}}^\dagger(\mathbf{q})\tilde{a}_{\text{NF}}(\mathbf{q}) + |\Delta(\mathbf{q})|^2 + 1 \right]. \quad (30.105)$$

The ground state of H^{NFG} is shifted from the vacuum energy $\sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}$ by an amount $\sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} |\Delta(\mathbf{q})|^2$. With a choice of metric leading to (30.102), the reader may verify from (30.77) and (30.78) that

$$\tilde{a}_0(\mathbf{q}) = -a_0^\dagger(\mathbf{q}) + 2\Delta^*(\mathbf{q}). \quad (30.106)$$

We know from the analysis in Sect. 30.3 that the Coulomb interaction between (fixed) charges can be interpreted as being due to exchange of scalar photons. In our previous approach thus only one photon type is needed in the description. In view of this one would expect that either the gauge photon or the near-field photon can be eliminated from the theory. To prove this, one makes use of the Gupta–Bleuler–Lorenz condition. This states that all physically acceptable states ($|\psi\rangle$) must satisfy the subsidiary condition in (29.112). It is important here to notice that the condition in this equation must hold even in the presence of field–matter interaction. By combination of (29.112) and (30.68) the Gupta–Bleuler–Lorenz condition can be expressed as a condition on the various modes, namely,

$$\left[iqa_L(\mathbf{q}) + \frac{1}{c_0}\dot{a}_0(\mathbf{q}) \right] |\psi\rangle = 0, \quad \forall \mathbf{q}. \quad (30.107)$$

The evolution equation for the scalar photon annihilation operator, i.e.,

$$i\hbar\dot{a}_0(\mathbf{q}) = [a_0(\mathbf{q}), H_S(\mathbf{q})], \quad (30.108)$$

now is used to simplify (30.107). By using the expression given in (30.76) for $H_S(\mathbf{q})$ one obtains

$$\begin{aligned} [a_0, H_S] &= \hbar\omega_{\mathbf{q}} \{ [a_0, -\tilde{a}_0 a_0] + \Delta [a_0, \tilde{a}_0] \} \\ &= \hbar\omega_{\mathbf{q}} \{ [\tilde{a}_0, a_0] a_0 + \Delta [a_0, \tilde{a}_0] \}. \end{aligned} \quad (30.109)$$

With the help of (29.146), the commutator finally is reduced to

$$\begin{aligned} [a_0(\mathbf{q}), H_S(\mathbf{q})] &= \hbar\omega_{\mathbf{q}} (a_0(\mathbf{q}) - \Delta(\mathbf{q})) \\ &= \hbar\omega_{\mathbf{q}} b_0(\mathbf{q}). \end{aligned} \quad (30.110)$$

The time-derivative of $a_0(\mathbf{q})$ thus is proportional to $b_0(\mathbf{q})$:

$$i\dot{a}_0(\mathbf{q}) = \omega_q b_0(\mathbf{q}). \quad (30.111)$$

On basis of (30.111) it appears that the subsidiary condition in (30.107) may be written as

$$[a_L(\mathbf{q}) - b_0(\mathbf{q})]|\psi\rangle = 0, \quad \forall \mathbf{q}. \quad (30.112)$$

Apart from a constant factor, the operator in (30.112) is our new near-field photon annihilation operator (see (30.97)). The Gupta–Bleuler–Lorenz condition

$$\tilde{a}_{\text{NF}}(\mathbf{q})|\psi\rangle = 0, \quad \forall \mathbf{q}, \quad (30.113)$$

therefore states that in the Coulomb interaction between two fixed charges only the displaced ground states of the near-field oscillators are of physical importance. In the Hamiltonian H^{NFG} (30.105) the near-field parts hence may be omitted from the outset. By utilizing (29.123) and (30.77) it is realized that the subsidiary condition in (30.112) may be written in a form

$$a_{\text{NF}}(\mathbf{q})|\psi\rangle = \frac{\Delta(\mathbf{q})}{i\sqrt{2}}|\psi\rangle, \quad \forall \mathbf{q}, \quad (30.114)$$

a result which states that all physical states involved in the Coulomb interaction are coherent states for the original(undisplaced) near-field part of the field. In the absence of charges ($\Delta(\mathbf{q}) = 0$) the subsidiary condition in (30.112) reduces to the free-field condition given in (29.113).

30.5 Classical Potentials Generated by a Prescribed Sheet Source

30.5.1 Sheet Current Density

In Chap. 4, the angular spectrum representation of classical electromagnetic fields was introduced and discussed, and the usefulness of the mixed Fourier transformation for the description of evanescent electromagnetic fields emphasized.

Let us now return to the sheet source concept, which plays such a central role in the angular spectrum representation. Using a slightly different notation from that of (4.55), the current density on a sheet located at $z = 0$ has the general form

$$\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) = \mathcal{J}(\mathbf{q}_{\parallel}, \omega)\delta(z) \quad (30.115)$$

in the mixed representation. In the following we will assume that $\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega)$ is a known (prescribed) function, and for simplicity the reference to $\mathbf{q}_{\parallel}$ and ω most often will be omitted from the notation, i.e., $\mathbf{J}(z; \mathbf{q}_{\parallel}, \omega) \equiv \mathbf{J}(z)$, and $\mathcal{J}(\mathbf{q}_{\parallel}, \omega) \equiv \mathcal{J}$. At this stage we allow the current density to have nonvanishing

components both parallel and perpendicular to the plane of the sheet. Since we aim at a field description in terms of transverse, longitudinal and scalar modes, the transverse and longitudinal parts of the sheet current density are needed. In the mixed representation these parts are generally given by

$$\mathbf{J}_I(z, \mathbf{q}_\parallel, \omega) = \int_{-\infty}^{\infty} \delta_I(z - z', \mathbf{q}_\parallel) \cdot \mathbf{J}(z'; \mathbf{q}_\parallel, \omega) dz' \quad (30.116)$$

with $I=T$ or L . In sheet (disk) contraction the longitudinal ($\delta_L(Z; \mathbf{q}_\parallel)$) and transverse ($\delta_T(Z; \mathbf{q}_\parallel)$) delta functions are given by [49]

$$\begin{aligned} \delta_L(Z; \mathbf{q}_\parallel) &= U\delta(Z) - \delta_T(Z; \mathbf{q}_\parallel) \\ &= \hat{z}\hat{z}\delta(Z) + \frac{q_\parallel}{2} e^{-iq_\parallel|Z|} [\hat{\mathbf{q}}_\parallel \hat{\mathbf{q}}_\parallel - \hat{z}\hat{z} + i(\hat{\mathbf{q}}_\parallel \hat{z} + \hat{z} \hat{\mathbf{q}}_\parallel) \operatorname{sgn} Z], \end{aligned} \quad (30.117)$$

where, for use in (30.116), $Z = z - z'$. By combining (30.115)–(30.117), it follows that the longitudinal part of the sheet current density is

$$\mathbf{J}_L(z) = \delta(z) \hat{z}\hat{z} \cdot \mathcal{J} + \theta(z) \mathcal{J}_L^> e^{-q_\parallel z} + \theta(-z) \mathcal{J}_L^< e^{q_\parallel z}, \quad (30.118)$$

where

$$\mathcal{J}_L^> = \frac{q_\parallel}{2} [\hat{\mathbf{q}}_\parallel \hat{\mathbf{q}}_\parallel - \hat{z}\hat{z} + i(\hat{\mathbf{q}}_\parallel \hat{z} + \hat{z} \hat{\mathbf{q}}_\parallel)] \cdot \mathcal{J}, \quad (30.119)$$

$$\mathcal{J}_L^< = \frac{q_\parallel}{2} [\hat{\mathbf{q}}_\parallel \hat{\mathbf{q}}_\parallel - \hat{z}\hat{z} - i(\hat{\mathbf{q}}_\parallel \hat{z} + \hat{z} \hat{\mathbf{q}}_\parallel)] \cdot \mathcal{J}. \quad (30.120)$$

It appears from (30.118) that $\mathbf{J}_L(z) \equiv \mathbf{J}_L(z; \mathbf{q}_\parallel, \omega)$ is nonvanishing also outside the sheet. The confinement of $\mathbf{J}_L(z; \mathbf{q}_\parallel, \omega)$ is exponential, and the spatial decay constant equals the magnitude of $\mathbf{q}_\parallel$. Outside the sheet the sum of the longitudinal and transverse parts of the current density is zero of course, i.e.,

$$\mathbf{J}_T(z; \mathbf{q}_\parallel, \omega) = -\mathbf{J}_L(z; \mathbf{q}_\parallel, \omega), \quad z \neq 0. \quad (30.121)$$

The sheet charge density, $\rho(z; \mathbf{q}_\parallel, \omega) \equiv c_0^{-1} J_0(z; \mathbf{q}_\parallel, \omega)$, which relates to the current density in (30.115), can be obtained from the equation of continuity, that is

$$\left(i\mathbf{q}_\parallel + \hat{z} \frac{\partial}{\partial z} \right) \cdot \mathbf{J}(z; \mathbf{q}_\parallel, \omega) = i\omega \rho(z; \mathbf{q}_\parallel, \omega) \quad (30.122)$$

in the mixed representation. Hence,

$$\rho(z) = \frac{1}{i\omega} \left(i\mathbf{q}_\parallel \cdot \mathcal{J} \delta(z) + \hat{z} \cdot \mathcal{J} \frac{d\delta(z)}{dz} \right), \quad (30.123)$$

a result which shows that the charge density has a term proportional to the first derivative of the delta function, but only if $\mathcal{J}$ has a component perpendicular to the plane of the sheet.

30.5.2 Longitudinal and Scalar Parts of the Classical Four-Potential

In near-field electrodynamics the longitudinal and scalar photons play an important role, and it is therefore of relevance to determine the classical scalar potential and the longitudinal part of the vector potential associated with the prescribed sheet current density in (30.115).

First, we study the longitudinal vector potential. In the mixed representation this is given by the integral expression

$$\mathbf{A}_L(z; \mathbf{q}_\parallel, \omega) = \mu_0 \int_{-\infty}^{\infty} g(z - z'; \mathbf{q}_\parallel, \omega) \mathbf{J}_L(z'; \mathbf{q}_\parallel, \omega) dz', \quad (30.124)$$

where

$$g(Z; \mathbf{q}_\parallel, \omega) = \frac{i}{2\kappa_\perp} e^{i\kappa_\perp |Z|} \quad (30.125)$$

is the scalar Green function studied in Sect. 4.3.1, and given already in (4.42). It is possible to carry out the integration in (30.124), but before this is done let me make a few general remarks. Although the charged particles are confined to a sheet, the source region of the longitudinal vector potential extends over a finite region of space in the present picture, namely the domain of $\mathbf{J}_L(z; \mathbf{q}_\parallel, \omega)$. From each z' -plane in this exponentially confined source region a field is generated. The field $\mathbf{A}_L(z)$ created at the observation plane $z = z$ by the infinitesimal source $\mathbf{J}_L(z') dz'$ is determined by the Green function $g(z - z')$. If the wave number $q_\parallel$ is smaller than the vacuum wave number $q_0 = \omega/c_0$, the created field is radiative [$\kappa_\perp = (q_0^2 - q_\parallel^2)^{1/2} > 0$], and $g(z - z')$ describes the field propagation. If instead $q_\parallel > q_0$, the generated field is of the evanescent type, since $\kappa_\perp = i\alpha_\perp$, where $\alpha_\perp = (q_\parallel^2 - q_0^2)^{1/2} > 0$.

Let us now turn our attention towards the calculation of $\mathbf{A}_L(z)$. By inserting (30.118) into (30.124) one obtains

$$\begin{aligned} \mathbf{A}_L(z) = \mu_0 \left[g(z) \hat{\mathbf{z}} \hat{\mathbf{z}} \cdot \mathcal{J} + \mathcal{J}_L^< \int_{-\infty}^0 g(z - z') e^{q_\parallel z'} dz' \right. \\ \left. + \mathcal{J}_L^> \int_0^{\infty} g(z - z') e^{-q_\parallel z'} dz' \right]. \end{aligned} \quad (30.126)$$

The first term on the right side of (30.126) originates in the singular part of the longitudinal current density (see (30.118)), and the second and third term stem from

the current densities located to the left ($z' < 0$) and right ($z' > 0$) side of the sheet, respectively. To proceed, it is useful to specify whether the plane of observation is to the left or right side of the sheet, and whether the generated field is propagating or evanescent. In the case where $z < 0$, the last integral in (30.126) becomes

$$\int_0^\infty g(z - z')e^{-q_\parallel z'} dz' = \frac{i e^{-i\kappa_\perp z}}{2\kappa_\perp(q_\parallel - i\kappa_\perp)}, \quad z < 0. \quad (30.127)$$

For $q_\parallel < q_0$, the longitudinal current density in the halfspace $z' > 0$ thus gives rise to a field propagating towards the left with a plane wave number $\kappa_\perp = (q_0^2 - q_\parallel^2)^{1/2}$. The result in (30.127) also holds for $q_\parallel > q_0$. With the replacement $\kappa_\perp = i\alpha_\perp$, it is clear that the field is evanescent and decays away from the sheet with a decay constant $\alpha_\perp$. In order to calculate the contribution to the field from the current density distribution in the halfspace $z' < 0$ one must divide the first integral in (30.126) into two parts since the Huygens propagator depends on the numerical value of $z - z'$. Thus,

$$\begin{aligned} \int_{-\infty}^0 g(z - z')e^{q_\parallel z'} dz' &= \frac{i}{2\kappa_\perp} \left[\int_{-\infty}^z e^{i\kappa_\perp(z-z')} e^{q_\parallel z'} dz' \right. \\ &\quad \left. + \int_z^0 e^{i\kappa_\perp(z'-z)} e^{q_\parallel z'} dz' \right], \quad z < 0, \end{aligned} \quad (30.128)$$

and then after a few elementary calculations we have

$$\int_{-\infty}^0 g(z - z')e^{q_\parallel z'} dz' = \frac{i e^{-i\kappa_\perp z}}{2\kappa_\perp(q_\parallel + i\kappa_\perp)} - \frac{e^{q_\parallel z}}{q_0^2}, \quad z < 0. \quad (30.129)$$

The last term in (30.129) is evanescent and decays in the direction $z \rightarrow -\infty$ with a decay constant $q_\parallel$. The first term is either propagating (towards the left) with a wave number $\kappa_\perp = (q_0^2 - q_\parallel^2)^{1/2}$ or evanescent with a decay constant $\alpha_\perp = (q_\parallel^2 - q_0^2)^{1/2}$, which is smaller than that of the last term. By inserting (30.127) and (30.129) into (30.126), we obtain the following result for the longitudinal vector potential when the plane of observation is located in the halfspace $z < 0$:

$$\begin{aligned} A_L(z) &= \mu_0 \left[\frac{i}{2\kappa_\perp} e^{-i\kappa_\perp z} \hat{z} \cdot \mathcal{J} - \frac{1}{q_0^2} e^{q_\parallel z} \mathcal{J}_L^< \right. \\ &\quad \left. + \frac{i}{2\kappa_\perp} e^{-i\kappa_\perp z} \left(\frac{\mathcal{J}_L^<}{q_\parallel + i\kappa_\perp} + \frac{\mathcal{J}_L^>}{q_\parallel - i\kappa_\perp} \right) \right], \quad z < 0, \quad q_\parallel < q_0. \end{aligned} \quad (30.130)$$

Although not necessary, it is useful for clarity to relate the result in (30.130) to the regime of propagation ($q_\parallel < q_0$), as indicated. With the replacement $\kappa_\perp \rightarrow i\alpha_\perp$, one obtains the explicit formula

$$\begin{aligned}
A_L(z) = \mu_0 \left[\frac{1}{2\alpha_\perp} e^{\alpha_\perp z} \hat{\mathbf{z}} \cdot \mathcal{J} - \frac{1}{q_0^2} e^{q_\parallel z} \mathcal{J}_L^< \right. \\
\left. + \frac{1}{2\alpha_\perp} e^{\alpha_\perp z} \left(\frac{\mathcal{J}_L^<}{q_\parallel - \alpha_\perp} + \frac{\mathcal{J}_L^>}{q_\parallel + \alpha_\perp} \right) \right], \quad z < 0, \quad q_\parallel > q_0
\end{aligned} \quad (30.131)$$

for the longitudinal vector potential in the evanescent ($q_\parallel > q_0$) regime. The reader may convince himself that the potential in the halfspace $z > 0$ can be obtained making the replacement $z \rightarrow -z$, and the interchange $\mathcal{J}_L^< \leftrightarrow \mathcal{J}_L^>$ in (30.130) and (30.131). Hence,

$$\begin{aligned}
A_L(z) = \mu_0 \left[\frac{i}{2\kappa_\perp} e^{i\kappa_\perp z} \hat{\mathbf{z}} \cdot \mathcal{J} - \frac{1}{q_0^2} e^{-q_\parallel z} \mathcal{J}_L^> \right. \\
\left. + \frac{i}{2\kappa_\perp} e^{i\kappa_\perp z} \left(\frac{\mathcal{J}_L^>}{q_\parallel + i\kappa_\perp} + \frac{\mathcal{J}_L^<}{q_\parallel - i\kappa_\perp} \right) \right], \quad z > 0, \quad q_\parallel < q_0,
\end{aligned} \quad (30.132)$$

and

$$\begin{aligned}
A_L(z) = \mu_0 \left[\frac{1}{2\alpha_\perp} e^{-\alpha_\perp z} \hat{\mathbf{z}} \cdot \mathcal{J} - \frac{1}{q_0^2} e^{-q_\parallel z} \mathcal{J}_L^> \right. \\
\left. + \frac{1}{2\alpha_\perp} e^{-\alpha_\perp z} \left(\frac{\mathcal{J}_L^>}{q_\parallel - \alpha_\perp} + \frac{\mathcal{J}_L^<}{q_\parallel + \alpha_\perp} \right) \right], \quad z > 0, \quad q_\parallel > q_0.
\end{aligned} \quad (30.133)$$

In analogy to (30.124), one may obtain the scalar potential in the mixed Fourier representation from the integral formula

$$A_0(z; \mathbf{q}_\parallel, \omega) = \mu_0 \int_{-\infty}^{\infty} g(z - z'; \mathbf{q}_\parallel, \omega) J_0(z'; \mathbf{q}_\parallel, \omega) dz', \quad (30.134)$$

inserting the expression given in (30.123) for $\rho(z'; \mathbf{q}_\parallel, \omega) = J_0(z'; \mathbf{q}_\parallel, \omega)/c_0$. With a preknowledge of $A_L(z; \mathbf{q}_\parallel, \omega)$, it is easier instead to use the Lorenz gauge condition, which in the mixed representation reads

$$A_0(z; \mathbf{q}_\parallel, \omega) = (iq_0)^{-1} \left(i\mathbf{q}_\parallel + \hat{\mathbf{z}} \frac{\partial}{\partial z} \right) \cdot \mathbf{A}_L(z; \mathbf{q}_\parallel, \omega). \quad (30.135)$$

For $z < 0$, one readily obtains, using (30.130), the temporary result

$$\begin{aligned}
A_0(z) = \frac{\mu_0}{iq_0} \left\{ \frac{\hat{\mathbf{z}} \cdot \mathcal{J}}{2} e^{-i\kappa_\perp z} - \frac{1}{q_0^2} (i\mathbf{q}_\parallel + q_\parallel \hat{\mathbf{z}}) \cdot \mathcal{J}_L^< e^{q_\parallel z} \right. \\
\left. + \frac{1}{2\kappa_\perp} \left[\frac{(\kappa_\perp \hat{\mathbf{z}} - \mathbf{q}_\parallel) \cdot \mathcal{J}_L^<}{q_\parallel + i\kappa_\perp} + \frac{(\kappa_\perp \hat{\mathbf{z}} - \mathbf{q}_\parallel) \cdot \mathcal{J}_L^>}{q_\parallel - i\kappa_\perp} \right] e^{-i\kappa_\perp z} \right\}. \quad (30.136)
\end{aligned}$$

Although combinations of the quantities $\mathcal{J}_L^<$ and $\mathcal{J}_L^>$ appear in (30.136), one must be able to express the result for $A_0(z)$ without use of these combinations, because the charge density is confined to the sheet plane ($z = 0$). To achieve this goal, one makes use of (30.119) and (30.120). Since

$$(i\mathbf{q}_\parallel + q_\parallel \hat{\mathbf{z}}) \cdot \mathcal{J}_L^< = 0, \quad (30.137)$$

there is no term proportional to $\exp(q_\parallel z)$ in (30.136). Utilizing the relations

$$\frac{(\kappa_\perp \hat{\mathbf{z}} - \mathbf{q}_\parallel) \cdot \mathcal{J}_L^<}{q_\parallel + i\kappa_\perp} = \frac{q_\parallel}{2} (-\hat{\mathbf{q}}_\parallel + i\hat{\mathbf{z}}) \cdot \mathcal{J}, \quad (30.138)$$

$$\frac{(\kappa_\perp \hat{\mathbf{z}} - \mathbf{q}_\parallel) \cdot \mathcal{J}_L^>}{q_\parallel - i\kappa_\perp} = \frac{q_\parallel}{2} (-\hat{\mathbf{q}}_\parallel - i\hat{\mathbf{z}}) \cdot \mathcal{J}, \quad (30.139)$$

it appears that the sum of the terms in the square bracket of (30.136) equals $-\mathbf{q}_\parallel \cdot \mathcal{J}$. Altogether, one obtains

$$A_0(z) = \frac{i\mu_0}{2\kappa_\perp q_0} e^{-i\kappa_\perp z} (\mathbf{q}_\parallel - \kappa_\perp \hat{\mathbf{z}}) \cdot \mathcal{J}, \quad z < 0, \quad q_\parallel < q_0, \quad (30.140)$$

in the case of propagating modes, and

$$A_0(z) = \frac{\mu_0}{2\alpha_\perp q_0} e^{\alpha_\perp z} (\mathbf{q}_\parallel - i\alpha_\perp \hat{\mathbf{z}}) \cdot \mathcal{J}, \quad z < 0, \quad q_\parallel > q_0 \quad (30.141)$$

for evanescent modes. I leave it as an exercise for the reader to show that the propagating and evanescent scalar potentials in the halfspace $z > 0$ are given by

$$A_0(z) = \frac{i\mu_0}{2\kappa_\perp q_0} e^{i\kappa_\perp z} (\mathbf{q}_\parallel + \kappa_\perp \hat{\mathbf{z}}) \cdot \mathcal{J}, \quad z > 0, \quad q_\parallel < q_0, \quad (30.142)$$

and

$$A_0(z) = \frac{\mu_0}{2\alpha_\perp q_0} e^{-\alpha_\perp z} (\mathbf{q}_\parallel + i\alpha_\perp \hat{\mathbf{z}}) \cdot \mathcal{J}, \quad z > 0, \quad q_\parallel > q_0, \quad (30.143)$$

respectively.

In the special case where the sheet current density lies in the plane of the sheet ($\hat{\mathbf{z}} \cdot \mathcal{J} = 0$), and in a direction perpendicular to the wave vector $\mathbf{q}_\parallel$ ($\hat{\mathbf{q}}_\parallel \cdot \mathcal{J} = 0$) both the scalar and longitudinal vector potential vanish. In a quantum electrodynamic context this means that no scalar and longitudinal photons can be generated by the sheet source.

30.5.3 Quasi-Static Regime

It is illuminating to discuss the longitudinal and scalar potentials in what might be called the quasi-static regime. We shall characterize this regime by two (approximate) requirements, which must be rigorously satisfied in the static limit. In this limit one cannot have a component of the sheet current density perpendicular to the plane of the sheet. Thus we take: (1) $\hat{\mathbf{z}} \cdot \mathcal{J} = 0$. In the quasi-static regime the field retardation is unimportant, and formally, the static limit is reached letting $c_0 \rightarrow \infty$. This implies that we have $q_{\parallel} > q_0 = \omega/c_0$ in the quasi-static regime. In turn this means that we always deal with evanescent modes in $A_L(z)$ and $A_0(z)$. As our second requirement we thus take: (2) $\alpha_{\perp} = q_{\parallel}$.

Let us proceed with some remarks on the longitudinal vector potential. For $z > 0$ and $q_{\parallel} > q_0$, the requirement $\hat{\mathbf{z}} \cdot \mathcal{J} = 0$ gives

$$A_L(z) = \frac{\mu_0}{2q_0^2} (\mathbf{q}_{\parallel} \cdot \mathcal{J}) \left[\left(\frac{q_{\parallel}}{\alpha_{\perp}} + i\hat{\mathbf{z}} \right) e^{-\alpha_{\perp}z} - (\hat{\mathbf{q}}_{\parallel} + i\hat{\mathbf{z}}) e^{-q_{\parallel}z} \right], \quad z > 0. \quad (30.144)$$

The corresponding result for $z < 0$ can be obtained making the replacements $\hat{\mathbf{z}} \rightarrow -\hat{\mathbf{z}}$ and $z \rightarrow -z$ in the equation above. Starting from (30.144), it appears that the requirement $\alpha_{\perp} = q_{\parallel}$ leads to

$$A_L(z; \mathbf{q}_{\parallel}, \omega) = \mathbf{0}, \quad (30.145)$$

a rigorous result only in the static limit. If needed one can of course obtain a finite quasi-static expression for $A_L(z)$ using the approximation $\alpha_{\perp}/q_{\parallel} \approx 1 - q_0^2/(2q_{\parallel}^2)$ in (30.144). To what extent the condition $\hat{\mathbf{z}} \cdot \mathcal{J} = 0$ can be upheld once $A_L(z)$ is nonvanishing is a difficult question to answer.

The requirement (1) and (2) lead immediately to the result

$$A_0(z; \mathbf{q}_{\parallel}, \omega) = \frac{\mu_0}{2q_0} (\hat{\mathbf{q}}_{\parallel} \cdot \mathcal{J}) e^{-q_{\parallel}z}, \quad z > 0, \quad (30.146)$$

for the scalar potential in the right halfspace. The replacement $z \rightarrow -z$ in (30.146) gives us $A_0(z)$ in the halfspace $z < 0$. Since the transverse vector potential vanishes in the static limit, i.e.,

$$A_T(z; \mathbf{q}_{\parallel}, \omega; c_0 \rightarrow \infty) = \mathbf{0}, \quad (30.147)$$

only scalar photons play a significant role in the quasi-static regime of electrodynamics. In this regime the Coulomb-like near-field interaction between two parallel current density sheets thus appears as resulting from an exchange of scalar photons. In the present context the Coulomb field originates in the spatial charge density modulation along the sheet, a modulation which exists whenever $q_{\parallel} \neq 0$. In the mixed representation the charge density is given by $\rho(z) = \omega^{-1}(\mathbf{q}_{\parallel} \cdot \mathcal{J})\delta(z)$; see (30.123).

30.5.4 Sheet Rim Zone

A knowledge of the longitudinal and scalar potentials allows one to determine the longitudinal part of the electric field in the mixed representation from

$$E_L(z) = i\omega A_L(z) - c_0 \left(i\mathbf{q}_{\parallel} + \hat{z} \frac{d}{dz} \right) A_0(z). \quad (30.148)$$

Using (30.145) and (30.146), one obtains for $z > 0$

$$E_L(z; \mathbf{q}_{\parallel}, \omega) = \frac{\mathbf{q}_{\parallel} \cdot \mathcal{J}}{2i\epsilon_0\omega} (\hat{\mathbf{q}}_{\parallel} + i\hat{z}) e^{-q_{\parallel}z} \quad (30.149)$$

in the limit $c_0 \rightarrow \infty$. The reader may readily verify that the quasi-static longitudinal field satisfies the rim zone condition

$$\left(i\mathbf{q}_{\parallel} + \hat{z} \frac{\partial}{\partial z} \right) \cdot E_L(z; \mathbf{q}_{\parallel}, \omega; c_0 \rightarrow \infty) = 0, \quad (30.150)$$

cf. (9.33), and the discussion in Sect. 9.2.2.

30.6 Quantum Field Radiated by a Classical Source

It is the purpose of a part of this last section of the book to extend the classical description just given of the field generated by a prescribed sheet source into the quantum regime.

30.6.1 Current Density Without Quantum Fluctuations

The quantum field radiated by a current density distribution $\{j_{\mu}(x)\}$ in general acts back on the current and affects it. In consequence the coupled field–matter problem becomes extremely difficult to solve in most cases. Here we assume that the radiation reaction is negligible, or compensated by some means. We further assume that the quantum fluctuations in the current density are negligible, i.e.,

$$\Delta j_{\mu}(x) = \left[\langle j_{\mu}^2(x) \rangle - (\langle j_{\mu}(x) \rangle)^2 \right]^{1/2} \approx 0. \quad (30.151)$$

For mesoscopic systems containing only a few mobile particles such an assumption can be difficult to satisfy, of course. A prescribed mean current density without significant quantum fluctuations we call a classical (cl) current density:

$$\{j_\mu(x)\} \Rightarrow \{j_\mu^{\text{cl}}(x)\} \equiv \{J_\mu(\mathbf{r}, t)\}. \quad (30.152)$$

In order to study the temporal quantum evolution of the global field–particle system only the state space of the electromagnetic field is needed when the currents are classical. In the covariant formulation of quantum electrodynamics the state space of the field can be considered to be the product of the subspaces of the transverse, longitudinal and scalar photons in a given inertial frame.

30.6.2 Heisenberg Equations of Motion for the Annihilation Operators $\{a_r(\mathbf{q}; t)\}$

In the Heisenberg picture, the evolution equation for the annihilation operator belonging to the polarization mode r (T1, T2, L, S) and the wave vector $\mathbf{q}$ has the form (cf. (23.97))

$$i\hbar\dot{a}_r(\mathbf{q}; t) = [a_r(\mathbf{q}; t), H], \quad (30.153)$$

where H is the Hamilton operator in (30.67). The commutator between a_r and the free-field part (H_F) of H is easily calculated. Since the annihilation and creation operators belonging to different $\mathbf{q}$ -modes commute (see (29.146) and (29.147)) we obtain

$$[a_r(\mathbf{q}; t), H_F] = \hbar\omega_q(-\zeta_r) [a_r(\mathbf{q}; t), \bar{a}_r(\mathbf{q}; t)a_r(\mathbf{q}; t)] \quad (30.154)$$

in the first step, and then

$$\begin{aligned} [a_r(\mathbf{q}; t), H_F] &= \hbar\omega_q(-\zeta_r) [a_r(\mathbf{q}; t), \bar{a}_r(\mathbf{q}; t)] a_r(\mathbf{q}; t) \\ &= \hbar\omega_q(-\zeta_r)^2 a_r(\mathbf{q}; t). \end{aligned} \quad (30.155)$$

The last member of (30.155) follows from (29.146). Hence, independent of the type of polarization mode one has

$$[a_r(\mathbf{q}; t), H_F] = \hbar\omega_q a_r(\mathbf{q}; t), \quad (30.156)$$

as expected. The calculation of the commutator between $a_r(\mathbf{q}; t)$ and the interaction Hamiltonian (H_I) is greatly simplified by the fact that a classical four-current density behaves like a c -number (H_I acts only on the field variables). Thus,

$$\begin{aligned} &\left[a_r(\mathbf{q}; t), \int_{-\infty}^{\infty} J_\mu(\mathbf{r}, t) A^\mu(\mathbf{r}, t) d^3r \right] \\ &= \int_{-\infty}^{\infty} J_\mu(\mathbf{r}, t) [a_r(\mathbf{q}; t), A^\mu(\mathbf{r}, t)] d^3r, \end{aligned} \quad (30.157)$$

remembering that summation over μ is implicit. A further reduction is obtained by inserting the expansion for $A^\mu(\mathbf{r}, t)$, given in (30.68), into (30.157), and using afterwards the commutation relations in (29.146) and (29.147). In this way one obtains

$$[a_r(\mathbf{q}; t), H_I] = \left(\frac{\hbar}{2\epsilon_0\omega_q L^3} \right)^{1/2} (-\zeta_r) \int_{-\infty}^{\infty} \epsilon_r^\mu J_\mu(\mathbf{r}, t) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r. \quad (30.158)$$

The commutator thus is a c -number, and the integral on the right side of (30.158) is the projection of the Fourier transformed classical four-current density

$$\{J_\mu(\mathbf{q}; t)\} = \int_{-\infty}^{\infty} \{J_\mu(\mathbf{r}, t)\} e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r, \quad (30.159)$$

on the polarization mode r . The results in (30.156) and (30.158) lead to the following evolution equation:

$$\dot{a}_r(\mathbf{q}; t) + i\omega_q a_r(\mathbf{q}; t) = s_r^{\text{cl}}(\mathbf{q}; t), \quad (30.160)$$

where

$$s_r^{\text{cl}}(\mathbf{q}; t) = i(2\epsilon_0\hbar\omega_q L^3)^{-1/2} \zeta_r J_\mu(\mathbf{q}; t) \epsilon_r^\mu. \quad (30.161)$$

To emphasize the classical character of $s_r(\mathbf{q}; t)$ it carries a superscript cl.

30.6.3 Coherent Field State

A classical source current necessarily has finite support in time, and we can therefore assume that the current density is zero everywhere in space before the time $t = 0$. We also assume that the charge density is zero for $t < 0$. The Heisenberg equation for $a_r(\mathbf{q}; t)$ thus has the solution

$$a_r(\mathbf{q}; t) = a_r(\mathbf{q}; 0) e^{-i\omega_q t} + \alpha_r(\mathbf{q}; t), \quad (30.162)$$

where

$$\alpha_r(\mathbf{q}; t) = \int_0^t s_r^{\text{cl}}(\mathbf{q}; t') e^{i\omega_q(t-t')} dt', \quad (30.163)$$

for $0 \leq t \leq T$, T being the time after which the source has stopped being active. The first term on the right-hand-side of (30.162) represents the free evolution of the quantum field $a_r(\mathbf{q}; 0)$, and the second term accounts for the source radiation.

Let us now assume that the electromagnetic field initially, i.e., before the source starts to radiate, is in the vacuum state

$$|\psi(0)\rangle = |0\rangle. \quad (30.164)$$

In the Heisenberg picture, this is also the state of the field for all later times; see Sect. 23.2.4. Since

$$a_r(\mathbf{q}; 0)|\psi(0)\rangle = 0 \quad (30.165)$$

for all r and $\mathbf{q}$, one obtains via (30.162)

$$a_r(\mathbf{q}; t)|0\rangle = \alpha_r(\mathbf{q}; t)|0\rangle. \quad (30.166)$$

The state $|0\rangle$ therefore is an eigenstate of the annihilation operator $a_r(\mathbf{q}; t)$ with the classical quantity (variable) $\alpha_r(\mathbf{q}; t)$ as eigenvalue. By acting with the unitary time evolution operator $U(t)$ on (30.166) we get

$$U(t)a_r(\mathbf{q}; t)U^\dagger(t)U(t)|\psi(0)\rangle = \alpha_r(\mathbf{q}; t)U(t)|\psi(0)\rangle. \quad (30.167)$$

The operator $U(t)a_r(\mathbf{q}; t)U^\dagger(t)$ is just the time independent annihilation operator in the Schrödinger picture (cf. (23.92)) viz., $a_r(\mathbf{q}; 0)$, and $U(t)|\psi(0)\rangle$ is the time dependent state vector in the same picture, i.e., $|\psi(t)\rangle$. Hence (30.167) becomes

$$a_r(\mathbf{q}; 0)|\psi(t)\rangle = \alpha_r(\mathbf{q}; t)|\psi(t)\rangle, \quad (30.168)$$

and this equation shows that the quantum state of the field at time t is a coherent state characterized by the complex number $\alpha_r(\mathbf{q}; t)$, which associates to the classical field from the source at the same time. Although the four-current density is classical the field is not completely so because it exhibits quantum fluctuations. In the coherent state these fluctuations are minimal in a certain sense [178].

30.6.4 Coherent Scalar and Longitudinal Photon Radiation from a Sheet Source

Let us now consider the field-quantized radiation problem from the classical sheet source described in Sect. 30.5.1. The perhaps most interesting part of the problem is that associated to the scalar and longitudinal photon radiation. For a prescribed sheet current density, assumed to have negligible quantum fluctuations, we know that the radiated field is in a globally coherent state. The main purpose here thus is to determine the complex coherence functions $\alpha_0(\mathbf{q}; t)$ and $\alpha_L(\mathbf{q}; t)$, cf. (30.161) and (30.163).

We start the calculation with the longitudinal photon field, for which the quantity $s_L^{\text{cl}}(\mathbf{q}; t)$ is given by

$$s_L^{\text{cl}}(\mathbf{q}; t) = iB\hat{\mathbf{q}} \cdot \mathbf{J}(\mathbf{q}; t), \quad (30.169)$$

because

$$\zeta_L J_\mu \epsilon_L^\mu = (-1)(-\mathbf{J}) \cdot \hat{\mathbf{q}} \quad (30.170)$$

for the L-mode. The quantity

$$B = (2\epsilon_0 \hbar \omega_q L^3)^{-1/2} \quad (30.171)$$

appears both for the longitudinal and scalar fields, and we already know its origin. The complete confinement of the current density in the z -direction implies that $\mathbf{J}(\mathbf{q}; t)$ is independent of $q_\perp$. Hence,

$$\mathbf{J}(\mathbf{q}; t) = \int_{-\infty}^{\infty} \mathcal{J}(\mathbf{q}_\parallel, \omega) e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (30.172)$$

The coherence function for the longitudinal photon field is obtained by integration of the quantity

$$s_L^{\text{cl}}(\mathbf{q}; t) = iB \int_{-\infty}^{\infty} \hat{\mathbf{q}} \cdot \mathcal{J}(\mathbf{q}_\parallel, \omega) e^{-i\omega t} \frac{d\omega}{2\pi} \quad (30.173)$$

between the times $t = 0$ and $t = t$; see (30.163). By inverting the integrals over time and frequency, the reader may show that

$$\alpha_L(\mathbf{q}; t) = c_0 B \int_{-\infty}^{\infty} \mathbf{q} \cdot \mathcal{J}(\mathbf{q}_\parallel, \omega) \frac{e^{-i\omega t} - e^{-i\omega_q t}}{\omega_q(\omega_q - \omega)} \frac{d\omega}{2\pi}, \quad (30.174)$$

remembering that $\hat{\mathbf{q}} = c_0 \mathbf{q} / \omega_q$.

To determine the coherence function for the scalar photon field, one must know the charge density in the $(\mathbf{q}; t)$ -domain. Utilizing the equation of continuity, which for the sheet takes the form

$$\rho(\mathbf{q}; \omega) = \omega^{-1} \mathbf{q} \cdot \mathcal{J}(\mathbf{q}_\parallel, \omega) \quad (30.175)$$

in the $(\mathbf{q}, \omega)$ -representation, one obtains

$$\rho(\mathbf{q}; t) = \int_{-\infty}^{\infty} \omega^{-1} \mathbf{q} \cdot \mathcal{J}(\mathbf{q}_\parallel, \omega) e^{-i\omega t} \frac{d\omega}{2\pi}. \quad (30.176)$$

From (30.161) we have

$$s_0^{\text{cl}}(\mathbf{q}; t) = iB c_0 \rho(\mathbf{q}; t), \quad (30.177)$$

and then by combination of (30.163) (for $r = 0$), (30.176), and (30.177), and integration over time, one finally gets the following coherence function for the scalar photon field:

$$\alpha_0(\mathbf{q}; t) = c_0 B \int_{-\infty}^{\infty} \mathbf{q} \cdot \mathcal{J}(\mathbf{q}_\parallel, \omega) \frac{e^{-i\omega t} - e^{-i\omega_q t}}{\omega(\omega_q - \omega)} \frac{d\omega}{2\pi}. \quad (30.178)$$

The reader should notice the close resemblance of the integral formulas for α_L (30.174) and α_0 (30.178). The difference between α_L and α_0 is given by

$$\begin{aligned}
& \alpha_L(\mathbf{q}; t) - \alpha_0(\mathbf{q}; t) \\
&= \frac{c_0}{(2\epsilon_0 \hbar \omega_q L^3)^{1/2}} \int_{-\infty}^{\infty} \mathbf{q} \cdot \mathcal{J}(\mathbf{q}_{\parallel}, \omega) \frac{e^{-i\omega_q t} - e^{-i\omega t}}{\omega \omega_q} \frac{d\omega}{2\pi} \quad (30.179)
\end{aligned}$$

in the time interval $[(0|T)]$ where the source is electro-dynamically active. Outside this interval both complex coherence functions have the time dependence characteristic for a free field, viz., $\exp(-i\omega_q t)$.

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