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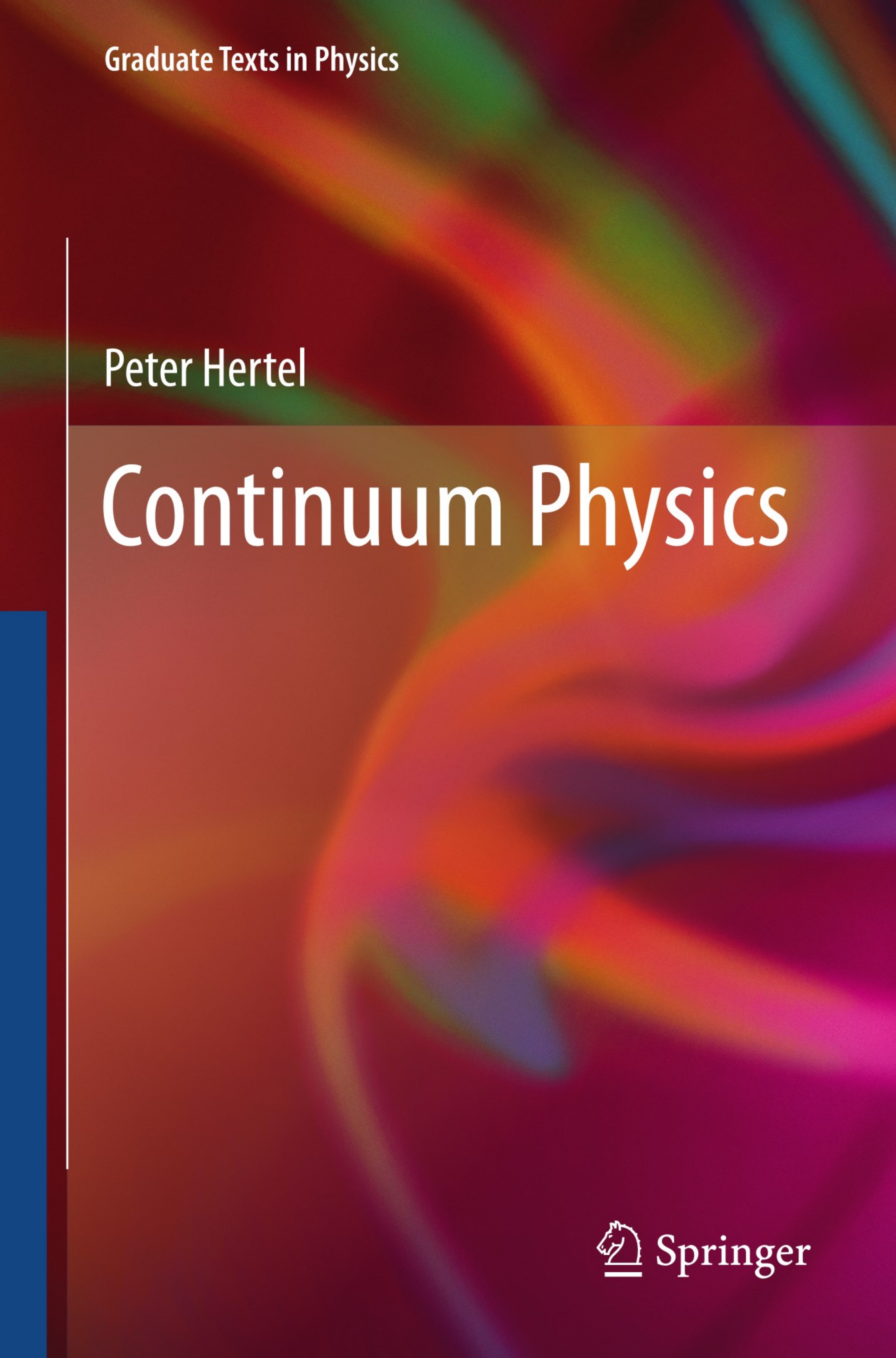

Peter Hertel

Continuum Physics

Springer

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Continuum Physics

With 37 Figures

Springer

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Preface

The subject of this small book is a vast field: continuum physics. Quite naturally, we cannot go into all the details of its many subdomains. Instead, we provide a bird's eye view of the subject .

A continuum is made up of material points. Each material point is a tiny region: tiny from a human point of view, where the natural scale are meters, kilograms, and seconds.

The same material point, however, contains very many particles, atoms or molecules, such that the statistical laws for infinitely many particles apply. In particular, external parameters change relatively slowly such that each material point is always very close to thermodynamic equilibrium.

Thus we deal with fields $f = f(t, \boldsymbol{x})$, where f stands for a property of the material point located at $\boldsymbol{x}$ at time t, such as mass density, temperature, tension, and so forth.

Chapter 1 discusses additive and transportable quantities such as mass, electric charge, momentum, kinetic, potential and internal energy as well as entropy. For each such quantity, a balance equation is formulated and related with other balance equations. Each quantity is described by densities for content, flow, and production. The balance equations must be respected in any case; they apply to all kinds of matter in any state. The highlights of this chapter are the precise formulations of the first and second main laws of thermodynamics in terms of partial differential equations.

Chapter 2 describes the special continuum under discussion with additional field equations, such as Hooke's law, Ohm's law, optical or acoustical properties, the ideal gas pressure relation, and so forth. Each closed set of field equations characterizes a subdomain of continuum physics: elasticity, hydrodynamics, aerodynamics, optics, rheology, thermo-electricity, diffusion, heat conduction, and so forth.

Next we study *Linear Response Theory* (Chap. 3). The reaction of a system in thermodynamic equilibrium to rapid variations of external parameters is worked out in first order perturbation theory. Linear material equations and explicit expression for their coefficients are arrived at, such as the dielectric susceptibility as a function of frequency. Once a tractable model for the system under consideration has been established, these coefficients can be calculated. Even more importantly, there are general relations, such as the Kramers-Kronig or Onsager relations, that can be shown to be true irrespective of a particular model. A highlight of this chapter is the derivation of the fluctuation-dissipation theorem, which is very close to a proof of the second main law of thermodynamics.

In Chap. 4, some standard topics of continuum physics are discussed. These examples serve to familiarize the reader with what she or he may already know, but now on a higher level, such as Archimedes' principle, the first article. Some topics, however, may be new to the reader. For instance, the last article presents a simplified model of a white dwarf. There are articles on crystal optics, the electro- and magneto-optic effect, and on optical activity as well as dielectric waveguides. Metamaterials and photonic crystals are also introduced. Standard problems of elasticity such as beam-bending and buckling, stress enhancement, and vibrating strings and membranes are discussed. The propagation and attenuation of sound waves in elastic bodies and in air as well as surface acoustic waves are dealt with. There is an article on surface plasmon polaritons, and we discuss Ohm's law and the Hall effect, introducing the Drude model. The reader will find sections on the laws of Bernoulli, Hagen-Poiseuille and Stokes and on Reynold's number. An article on local chemical reactions and diffusion introduces the interesting subject of pattern formation. Fourier's classical treatment of a heat conduction problem is presented and thermoelastic effects explained (Thomson, Seebeck, Peltier). Two articles illustrate the dissipation-fluctuation theorem: one on the thermal noise of an Ohmic resistor, and the other on various aspects of Brownian motion. Diffusion, a standard subject in continuum physics, is nothing else but mass-wise Brownian motion. A model of the earth's atmosphere is also discussed.

Chapter 4 could also have been organized into a series of methods of solving partial differential equations. Some can be solved analytically exploiting symmetry, others by rewriting them into systems of ordinary differential equations. The articles on Stokes' law and on stress concentration introduce the potential method. Various Computational schemes such as the finite difference method and the finite element method are also discussed. The sample programs presented are in `MATLAB` because this software package is tailored to the needs of physics.

An appendix covers *Fields*: their transformation properties, how they are differentiated and how they can be integrated over paths, areas, and volumes. After all, continuum physics is formulated in terms of fields and relations between them. There is also a *Glossary*, which may serve as a summary of this bird's eye view of continuum physics. It provides brief descriptions of the main topics of this book and lists most of the people who have entered the stage.

The book systematically presents continuum physics theory (balance equations, material equations, linear response) and substantiates the theory with selected examples. Both parts are of comparable size. On the one hand, the examples cannot be understood without a solid theoretical foundation. On the other hand, physical laws as such are without pertinence if they cannot be shown to be useful for real-world problems—from Archimedes' principle to white dwarfs.

This book can be read in practically any order. It is more like a web than an exposition where the next step cannot be taken without going over all the previous steps. However, the first few sections on balance equations should be read first and consecutively because they introduce a precise system of notation that is nevertheless more or less compatible with a century-old tradition.

This book on *Continuum Physics* addresses students of physics, engineering, and related branches of science with a general background in calculus and basic physics. It will also serve graduate students and lecturers who want to embed their special field in a wider context.

The book presents the physics of continuously distributed matter in a unified way. We have built and developed a stringent theoretical framework and discussed carefully chosen examples. This will enable the reader to assemble the multitude of principles, rules, laws, effects, and theories of continuum physics—the pieces of a jigsaw puzzle—into a coherent whole.

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February 2012

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Chapter 1
Balance Equations

In this chapter we discuss physical quantities like mass, electric charge, energy and so on. If two systems are joined, these quantities add. The quantities in question are bound to particles, atoms or molecules. If they move, they take their properties with them. Therefore the quantities under discussion are transportable.

Central to continuum physics is the idealization of *Material points*. It is a good approximation for very many situations to assume that a region of space can be divided into cells which are quasi infinitely small on a macroscopic scale and quasi infinitely large on a microscopic scale. We argue why this is no contradiction.

In section *Densities for content, flow and production rate* we introduce, for each additive and transportable quantity, a density, a current density, and a volumetric production rate. The general balance equation states that the amount of a quantity within a region might increase because there is more inflow than outflow of this quantity across the surface or because the quantity is produced within the region.

Next we apply this to particles which come in species. The particles of the same species are indistinguishable, so we will never enumerate them, we only speak of how many there are. Since each particle carries a mass and an electric charge with it, we arrive quite naturally at the appropriate conservation laws. This is the content of section *Particle numbers, mass, and electric charge*.

It is now appropriate to discuss the transformation behavior of the current densities. We must split them into a *convection and a conduction* contribution such that the latter transforms as a vector field, i.e., does not depend on the velocity of the observer. We discuss the consequences for particle numbers, mass, and electric charge.

Momentum can be transported because particles move, thereby carrying their momentum with it, and by short range interactions. The latter effect is described by the stress tensor. We will see that this tensor field should normally be symmetric.

Energy is conserved. We distinguish between kinetic, potential, and internal energy which separately are not conserved. We arrive at a balance equation for the internal energy which is a very precise formulation of the first law of thermodynamics in terms of partial differential equations.

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Entropy is not conserved. We expand the idea that each material point, because it is so small, is always almost in thermodynamic equilibrium. The parameters, however, which describe this local equilibrium, vary from place to place, such that normally there is no global equilibrium. The production rate of entropy per unit volume, for which we develop a concrete expression, is never negative. This statement is the second main law of thermodynamics.

1.1 Material Points

The notion of a material point is central to continuum physics. Such a material point is a region of space, a cube say, which is so small that it appears as a point to the engineer. On the other hand, the same material point contains so many atoms or molecules that one may speak of a large thermodynamic systems. These two characterizations do not contradict each other, as we will show now.

Let us discuss an example. The material point shall be 1 mm × 1 mm × 1 mm. Its volume is $V = 10^{-9}\,\mathrm{m}^3$. Think of an ideal gas under normal conditions.[1] One mole is made up of $6.022141 \times 10^{23}\,\mathrm{mol}^{-1}$ molecules, it occupies a volume of 22.4 L. Hence, the material point contains $N = 2.7 \times 10^{16}$ particles. This is a huge number, in fact, it is sufficiently close to infinity so that the thermodynamic limit is applicable.

Thermodynamic laws are derived for N particles in a region of volume V, and by sending $N, V \to \infty$ such that the particle density $n = N/V$ remains constant. The pressure law $p = nk_{\mathrm{B}}T$ is an example: the pressure p of an ideal gas is proportional to the particle density n and the absolute temperature T. k_{B} is Boltzmann's constant.[2] Only if N is large enough we can rely on $pV = Nk_{\mathrm{B}}T$. And N for the material point which we have described above is certainly large enough.

But there is more to it. Our material point is an open region. Particles may come in and may go out. In fact, the number N of particles within the material point is an observable. Above we have calculated the average number $\bar{N} = \langle N \rangle$ of particles within the material point under consideration.

For an ideal gas one finds $\langle N^2 \rangle = \langle N \rangle^2 + \langle N \rangle$. The root mean square fluctuation is defined by $\delta N = \sqrt{\langle N^2 \rangle - \langle N \rangle^2}$. We just have seen that for an ideal gas $\delta N = \sqrt{\bar{N}}$ holds true. The relative root mean square fluctuation $\delta N/\bar{N}$ diminishes as $1/\sqrt{\bar{N}}$ for larger and larger systems.

Our model material point contains 2.7×10^{16} particles on the average, the relative fluctuations therefore are of order 10^{-8}. This value is small enough to be neglected.

We have just shown that, for an ideal gas under normal conditions, a small cube of volume V contains so many molecules N that the thermodynamic limit is applicable

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[1] Pressure 1,013 hPa, 0°C temperature.

[2] $k_{\mathrm{B}} = 1.380649 \times 10^{-23}\,\mathrm{J\,K}^{-1}$.

for $n = N/V$ and that fluctuations can safely be neglected. On the other hand, the system is small enough so that the material point will rapidly reach thermodynamic equilibrium. Thus, if t denotes time and $\boldsymbol{x} = (x_1, x_2, x_3)$ is the center of the material point, we may speak of $n = n(t, \boldsymbol{x})$, the particle density now and here. This is a real-valued function of time and space, a classical field.

Similar considerations apply to other quantities, like pressure or internal energy, and to other systems such as liquids or solids. We have made plausible that sufficiently small regions, which appear as a point to the engineer, are large enough to be described by statistical thermodynamics. This compromise between small from the engineer's point of view, and large as judged by statistical physics—this is the essence of continuum physics. We shall later discuss this in more detail.

In the language of mathematics, a point is an object without internal structure. Vectors can be points, and functions as well. Material points in this sense have properties like location with respect to a coordinate system, mass density, temperature, electrical field strength, and so forth. In the same sense, a vector will have a length, and a function an attribute like continuous or a value such as an integral. In the context of continuum physics, it makes no sense to speak of the center of a material point or of its boundary or volume. Continuum physics is embedded into classical and quantum mechanics and statistical physics. One thinks and argues in terms of particles $i = 1, 2, \dots, N$ of species a with mass m_a, charge q_a at location $\boldsymbol{x}_i$ and so forth in order to *derive* the laws of continuum physics. But these laws will be formulated in terms of classical fields, such as the particle density $n^a = n^a(t, \boldsymbol{x})$. At time t and at location $\boldsymbol{x}$ there are n^a particles of species a per unit volume. Put otherwise, the material point at $\boldsymbol{x}$ is characterized by an a-particle density $n^a(t, \boldsymbol{x})$, at time t, and by many more such field values.

The collection of material points form a continuum, and one may speak of neighboring points. In fact, the notion of differential quotients is a valid idealization. The fields by which a continuum is described have gradients, or a divergence, or a curl, and also time derivatives. Continuum physics is described by partial differential equations and by local relations between properties of material points.

1.1.1 Summary

The notion of a material point is central to continuum physics. Regions which appear as points to the engineer contain nevertheless so many particles that formulas of statistical physics may be applied which describe the limit of infinitely many particles. Statistical fluctuations can safely be neglected. The collection of material points is a continuum, its properties are described by fields $f = f(t, \boldsymbol{x})$ and partial differential equations as well as local relations involving these fields.

1.2 Densities for Content, Flow, and Production Rate

Let us denote by Y an additive, transportable quantity. Number of particles, mass, electric charge, momentum, internal energy or entropy are examples. We talk about them in the following sections. Here we want to introduce spatial densities, current densities and volumetric production rates for such additive and transportable quantities, and the generic balance equation.

1.2.1 Densities

Denote by $\mathcal{V}$ a region of three-dimensional space, a ball or a cube say. We call it a volume, although the same word is used for its content

$$\mathrm{vol}(\mathcal{V}) = \int_{\mathcal{V}} \mathrm{d}V. \tag{1.1}$$

$\mathrm{d}V$ is the volume element. See Appendix A for paths, surfaces and volumes and the corresponding integrals of fields.

We denote by $Q(Y;t,\mathcal{V})$ the content of quantity Y within the volume $\mathcal{V}$ at time t. Y is an additive quantity if

$$Q(Y;t,\mathcal{V}_1 \cup \mathcal{V}_2) = Q(Y;t,\mathcal{V}_1) + Q(Y;t,\mathcal{V}_2) \tag{1.2}$$

holds true for arbitrary disjoint volumes $\mathcal{V}_1$, $\mathcal{V}_2$, $\mathcal{V}_1 \cap \mathcal{V}_2 = \emptyset$.

Volume obviously is an additive quantity. We shall argue in the next section why the number of particles of a certain species is additive as well and quantities derived from it.

Relation (1.2) can be generalized to a decomposition of a volume $\mathcal{V}$ into material points of infinitesimal volume $\mathrm{d}V$. We will write

$$Q(Y;t,\mathcal{V}) = \int_{\mathcal{V}} \mathrm{d}V\, \varrho(Y;t,\boldsymbol{x}). \tag{1.3}$$

$\varrho(Y;t,\boldsymbol{x})$ is the density of quantity Y at time t at the location $\boldsymbol{x}$. It has the physical dimension of Y quantity per unit volume.

1.2.2 Current Densities

Let $\mathcal{A}$ be an oriented surface. This is a two dimensional manifold with well defined front and back side. The well-known Möbius strip is *not* oriented. The surface of a sphere is oriented. Points close to the surface are either inside the sphere, at the back side of the surface, or outside, at the front side.

At a certain point $\boldsymbol{x} \in \mathcal{A}$ we have a positive surface element $\mathrm{d}A$ and a unit vector $\boldsymbol{n}$ which is normal to the surface and points from the back side towards the front side. The area of the surface is defined by

$$\text{area}(\mathcal{A}) = \int_{\mathcal{A}} \mathrm{d}A. \tag{1.4}$$

The surface integral of a vector field $\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{x})$ is written as

$$\int_{\mathcal{A}} \mathrm{d}A\, \boldsymbol{n} \cdot \boldsymbol{V}. \tag{1.5}$$

The field strength $\boldsymbol{V}$ is projected onto the surface normal $\boldsymbol{n}$, multiplied by $\mathrm{d}A$, and the infinitesimal contributions are added up. It is common practice to write $\mathrm{d}\boldsymbol{A} = \mathrm{d}A\, \boldsymbol{n}$ such that (1.5) reads

$$\int_{\mathcal{A}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{V}. \tag{1.6}$$

Let us denote by $I(Y; t, \mathcal{A})$ the net amount of quantity Y which passes, per unit time, from the back to the front side of the surface. This amount will depend on time t. The current should be a surface integral for which we write

$$I(Y; t, \mathcal{A}) = \int_{\mathcal{A}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{j}(Y; t, \boldsymbol{x}). \tag{1.7}$$

$\boldsymbol{j}(Y) = \boldsymbol{j}(Y; t, \boldsymbol{x})$ is the current density associated with the additive and transportable quantity Y.

The current density $\boldsymbol{j}(Y)$ indicates magnitude and direction of the local flow of Y. Its physical dimension is Y quantity per unit time per unit area.

$\mathrm{d}\boldsymbol{A} \cdot \boldsymbol{j}(Y) = \mathrm{d}A\, \boldsymbol{n} \cdot \boldsymbol{j}(Y)$ says that the current density has to be projected onto the normal of the surface element $\mathrm{d}A$. The current density can be decomposed into a contribution normal and parallel to $\mathrm{d}\boldsymbol{A}$. Only the normal component contributes to the passage of Y from the back to the front side.

If $\mathrm{d}\boldsymbol{A} \cdot \boldsymbol{j}(Y)$ is positive, then Y effectively flows from the back side to the front side. $\mathrm{d}\boldsymbol{A} \cdot \boldsymbol{j}(Y) < 0$ means that Y effectively flows from the front to the back side.

1.2.3 Production

An additive and transportable quantity Y may be produced or annihilated. Think of electric field energy which may vanish because it is converted into internal energy, or heat. Likewise the momentum content of a volume may be increased by external forces.

Let us denote by $\Pi(Y;t,\mathcal{V})$ the net amount of Y produced per unit time within the volume $\mathcal{V}$. This production rate may depend on time t.

We shall represent the production rate as a volume integral of production rates for material points:

$$\Pi(Y;t,\mathcal{V}) = \int_{\mathcal{V}} \mathrm{d}V\, \pi(Y;t,\boldsymbol{x}). \tag{1.8}$$

$\pi(Y) = \pi(Y;t,\boldsymbol{x})$ is the volumetric production rate for the quantity Y, at time t, at location $\boldsymbol{x}$. *Volumetric* in this context means *per unit volume*. Source strength is another name for $\pi(Y) = \pi(Y;t,\boldsymbol{x})$.

1.2.4 Generic Balance Equation

Consider a volume $\mathcal{V}$ with its surface $\partial\mathcal{V}$. We argue that the amount of Y within $\mathcal{V}$ will change because Y flows in through the surface $\partial\mathcal{V}$ or is produced within $\mathcal{V}$:

$$\frac{\mathrm{d}Q(Y;t,\mathcal{V})}{\mathrm{d}t} = -I(Y;t,\partial\mathcal{V}) + \Pi(Y;t,\mathcal{V}). \tag{1.9}$$

This balance equation is valid at all times t and for any volume $\mathcal{V}$.

We now invoke Gauss' theorem:

$$\int_{\partial\mathcal{V}} \mathrm{d}\boldsymbol{A}\cdot\boldsymbol{V} = \int_{\mathcal{V}} \mathrm{d}V\, \nabla\cdot\boldsymbol{V}. \tag{1.10}$$

It is valid for any reasonable volume $\mathcal{V}$ and for any piecewise differentiable vector field $\boldsymbol{V} = \boldsymbol{V}(t,\boldsymbol{x})$. $\nabla\cdot\boldsymbol{V}$ is the divergence of $\boldsymbol{V}$.

We insert this into (1.9) and obtain

$$\int_{\mathcal{V}} \mathrm{d}V\, \{\, \dot{\varrho}(Y) + \nabla\cdot\boldsymbol{j}(Y) - \pi(Y)\,\} = 0. \tag{1.11}$$

$\dot{\varrho}(Y) = \dot{\varrho}(Y;t,\boldsymbol{x})$ is the partial derivative of the density $\varrho(Y)$ with respect to time. Since Eq. (1.11) holds true for an arbitrary volume $\mathcal{V}$, the integrand has to vanish at any time and at any location,

$$\dot{\varrho}(Y,t,\boldsymbol{x}) + \nabla\cdot\boldsymbol{j}(Y;t,\boldsymbol{x}) = \pi(Y;t,\boldsymbol{x}). \tag{1.12}$$

This is the generic balance equation for an additive and transportable quantity Y on which we will elaborate in the following sections. It must be fulfilled at any time and everywhere, it is a field equation. We therefore abbreviate Eq. (1.12) to

$$\dot{\varrho}(Y) + \nabla\cdot\boldsymbol{j}(Y) = \pi(Y). \tag{1.13}$$

With ∂_t as partial derivative with respect to time and ∂_i as partial derivative with respect to the ith spatial coordinate, Eq. (1.13) may be rewritten as

$$\partial_t \varrho(Y) + \sum_{i=1,2,3} \partial_i j_i(Y) = \pi(Y). \tag{1.14}$$

Later we will even drop the summation symbols. If in one and the same expression a spatial index appears twice, summation over it is understood automatically.[3] Thus, Eqs. (1.12)–(1.14) now read

$$\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y). \tag{1.15}$$

The symbol i in the above equation is dummy, it does not appear in the result. $\partial_t \varrho(Y) + \partial_k j_k(Y) = \pi(Y)$ is the same as Eq. (1.15).

Let us add a word of caution. Replace $j_i(Y)$ by $j_i'(Y)$ and $\pi(Y)$ by $\pi'(Y) - \partial_i j_i(Y)$. Then both balance equations

$$\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y) \;\text{ and }\; \partial_t \varrho(Y) + \partial_i j_i'(Y) = \pi'(Y) \tag{1.16}$$

hold true. The distinction between inflow and production of Y is ambiguous. Any definition of a current density must be justified by physical, not only formal reasoning.[4]

1.2.5 Summary

An additive and transportable quantity Y is locally described by its density $\varrho(Y)$, a current density $\boldsymbol{j}(Y)$, and by a volumetric production rate $\pi(Y)$. These fields are related by the generic balance equation which states that the content increases if there is a net inflow and/or production. Equations (1.12)–(1.15) describe this simple consideration by formulas of increasing abstraction. However, the distinction between inflow and production is not unique, it must be substantiated by physical insight.

---

[3] Einstein's summation convention.

[4] A well-known example is the expression for the Poynting vector $\boldsymbol{j}(E^{\text{em}}) = \boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ for the energy E^{em} of an electromagnetic field. Many alternative forms have been proposed such that the energy current density is restricted to regions where electric charge flows. However, none of the alternatives is compatible with the notion that field energy is transported by streams of photons.

1.3 Particle Numbers, Mass, and Electric Charge

In this section we elaborate on particles and on properties carried by them. Particles of the same species, like protons or water molecules, are indistinguishable. Only their number within a specified regions makes sense, but not where they are located individually. Particles may vanish or appear in chemical reactions which are described by stoichiometric coefficients. The balance equation for the number of particles of a certain species is derived. Conservation laws for mass and electric charge are consequences because these quantities are conserved at the atomic level.

1.3.1 Particle Numbers and Currents

We mark the species of particles by an index a. For example, let us discuss water. There are H_2O molecules ($a = 1$), H^+ ions ($a = 2$), OH^- ions ($a = 3$), H_2 molecules ($a = 4$) as well as O_2 molecules ($a = 5$). N^a, the number of particles of species a, are additive and transportable quantities.

The density of particles of species a is

$$\varrho(N^a) = n^a = n^a(t, \boldsymbol{x}). \tag{1.17}$$

If there are no particles, they cannot flow. Hence, $n^a = 0$ always means $\boldsymbol{j}(N^a) = 0$. $\boldsymbol{j}(N^a) \neq 0$ is impossible with $n^a = 0$. Therefore, we may divide the particle current density (where it does not vanish) by the particle density. Put otherwise, we may write

$$\boldsymbol{j}(N^a) = n^a \, \boldsymbol{v}^a, \tag{1.18}$$

where $\boldsymbol{v}^a = \boldsymbol{v}^a(t, \boldsymbol{x})$ is to be interpreted as the average local velocity of particles of species a, at location $\boldsymbol{x}$, at time t.

1.3.2 Chemical Reactions

The number of particles of a certain species is *not* conserved. Particles may vanish and appear in chemical reactions.

Let us label by $r = 1, 2, \dots$ the possible chemical reactions. If one reaction of type r takes place, then ν^{ra} particles of species a will be created or annihilated, depending on the sign.

Table 1.1 may serve as an example. The ν^{ra} are *stoichiometric coefficients*. The rows in this table must not have a common divisor.

Denote by Γ^r the number of chemical reactions of type r, per unit time and unit volume. There is no commonly accepted name for it, we call it a *volumetric reaction rate*.

Table 1.1 Chemical reactions of water molecules. $a = 1, 2, \dots 5$ enumerates the particles involved. $r = 1, 2$ labels the reactions. The integer numbers are stoichiometric coefficients

ν^{ra}	Particle a	H_2O	H^+	OH^-	H_2	O_2
Reaction r		(1)	(2)	(3)	(4)	(5)
$H_2O \rightarrow H^+ + OH^-$	(1)	−1	1	1	0	0
$2H_2O \rightarrow 2H_2 + O_2$	(2)	−2	0	0	2	1

With this in mind we may write

$$\pi(N^a) = \pi^a = \sum_r \Gamma^r \nu^{ra}. \tag{1.19}$$

To summarize: The balance equation for particles of species a reads

$$\partial_t n^a + \partial_i n^a v_i^a = \sum_r \Gamma^r \nu^{ra}. \tag{1.20}$$

$n^a = n^a(t, \boldsymbol{x})$ is the density of particles of species a, $v_i^a = v_i^a(t, \boldsymbol{x})$ their average velocity. $\Gamma^r = \Gamma^r(t, \boldsymbol{x})$ denotes the number of chemical reactions of type r, per unit time and unit volume. The stoichiometric coefficients ν^{ra} are small integer numbers. Each chemical reaction of type r will produce ν^{ra} particles of species a. Note that n^a, v_i^a, and Γ^r are fields which depend on time and location. Also note that we apply Einstein's summation convention. $\partial_i n^a v_i^a$ stands for $\partial_1 n^a v_1^a + \partial_2 n^a v_2^a + \partial_3 n^a v_3^a$, the divergence of the particle current density.

1.3.3 Mass

Mass is the prototype of an additive and transportable quantity which we denote by M. We follow tradition and abbreviate the mass density $\varrho(M)$ by ϱ. It is related with particle densities by the following expression:

$$\varrho = \sum_a m^a n^a. \tag{1.21}$$

m^a is the mass of a single a-particle.

The mass current density is

$$j_i(M) = \sum_a m^a j_i(N^a) = \sum_a m^a n^a v_i^a. \tag{1.22}$$

We define the flow velocity $\boldsymbol{v}$ by setting

$$j_i(M) = \varrho v_i. \tag{1.23}$$

This is allowed since there cannot be a mass current without mass.[5]

Let us compare Eq. (1.22) with Eq. (1.23):

$$\boldsymbol{v} = \sum_a \frac{m^a n^a}{\varrho}\, \boldsymbol{v}^a. \tag{1.24}$$

Obviously the flow velocity is an average over particle flow velocities. The weight of species a is its contribution to the mass density.

Let us now discuss the mass production rate

$$\pi(M) = \sum_a m^a \pi(N^a). \tag{1.25}$$

We refer to Eq. (1.19) and obtain

$$\pi(M) = \sum_{ar} m^a \Gamma^r \nu^{ra}. \tag{1.26}$$

Mass is conserved for each individual reaction.[6] This finding is expressed by

$$\sum_a m^a \nu^{ra} = 0. \tag{1.27}$$

Inserted into Eq. (1.26), this results in $\pi(M) = 0$. The volumetric production rate of mass vanishes. Mass is conserved.

To summarize: the mass balance equation reads

$$\partial_t \varrho + \partial_i \varrho v_i = 0. \tag{1.28}$$

$\varrho = \varrho(t, \boldsymbol{x})$ denotes the mass density and $\boldsymbol{v} = \boldsymbol{v}(t, \boldsymbol{x})$ the flow velocity of the continuum under consideration.

1.3.4 Electric Charge

Besides mass, particles carry an electric charge. A particle of species a carries an electric charge q^a which is an integer multiple of the elementary charge e.

Electric charge, which we denote by Q^{e}, is another example of an additive and transportable physical quantity.

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[5] As opposed to charge, where there may be a charge current density while the charge density vanishes.

[6] At least in non-relativistic approximation.

We abbreviate the electric charge density by $\varrho^{\mathrm{e}} = \varrho(Q^{\mathrm{e}})$. It is defined by

$$\varrho^{\mathrm{e}} = \sum_a q^a n^a \tag{1.29}$$

in terms of particle densities.

Likewise the electric current density is defined as

$$\boldsymbol{j}^{\mathrm{e}} = \sum_a q^a \boldsymbol{j}(N^a) = \sum_a q^a n^a \boldsymbol{v}^a. \tag{1.30}$$

The volumetric production rate is

$$\pi(Q^{\mathrm{e}}) = \sum_a q^a \pi(N^a) = \sum_{ar} q^a \Gamma^r \nu^{ra}. \tag{1.31}$$

Electric charge is conserved for each individual reaction. This finding is expressed by

$$\sum_a q^a \nu^{ra} = 0. \tag{1.32}$$

Therefore Eq. (1.31) results in

$$\pi(Q^{\mathrm{e}}) = 0. \tag{1.33}$$

Electric charge, like mass, is not produced or annihilated, it is merely redistributed.

We summarize this:

$$\partial_t \varrho^{\mathrm{e}} + \partial_i j_i^{\mathrm{e}} = 0. \tag{1.34}$$

In the context of electromagnetism, Eq. (1.34) is called the continuity equation for electric charge.

1.3.5 Digression on Electromagnetism

The electromagnetic field is produced by electrically charged particles, and it is also felt only by them. A particle of mass m, charge q and momentum $\boldsymbol{p}$ experiences a force

$$\dot{\boldsymbol{p}} = q\{\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\}. \tag{1.35}$$

$\boldsymbol{E}$ is the electric field strength, $\boldsymbol{B}$ the magnetic induction. The momentum $\boldsymbol{p}$ of the particle and its velocity $\boldsymbol{v}$ are related by

$$\boldsymbol{p} = \frac{m\boldsymbol{v}}{\sqrt{1 - v^2/c^2}}, \tag{1.36}$$

where c is the speed of light in vacuum.

The electromagnetic field $\boldsymbol{E}, \boldsymbol{B}$ itself is generated by the density and current density of electric charge:

$$\epsilon_0 \nabla \cdot \boldsymbol{E} = \varrho^{\mathrm{e}}, \tag{1.37}$$

$$\frac{1}{\mu_0} \nabla \times \boldsymbol{B} - \epsilon_0 \dot{\boldsymbol{E}} = \boldsymbol{j}^{\mathrm{e}}. \tag{1.38}$$

There are two more equations for the electromagnetic field, namely

$$\nabla \cdot \boldsymbol{B} = 0 \tag{1.39}$$

and

$$\nabla \times \boldsymbol{E} + \dot{\boldsymbol{B}} = 0, \tag{1.40}$$

which state that there is no magnetic charge. ϵ_0 and μ_0 are constants which depend on the system of units. Equations (1.37)–(1.40) are Maxwell's equations.

Differentiating Eq. (1.37) with respect to time and adding the divergence of Eq. (1.38) yields

$$\dot{\varrho}^{\mathrm{e}} + \nabla \cdot \boldsymbol{j}^{\mathrm{e}} = \epsilon_0 \nabla \cdot \dot{\boldsymbol{E}} + \frac{1}{\mu_0} \nabla \cdot (\nabla \times \boldsymbol{B}) - \epsilon_0 \nabla \cdot \dot{\boldsymbol{E}} = 0. \tag{1.41}$$

The first and the last term on the right hand side cancel, and the term in the middle vanishes as well since it is the divergence of a curl. Conservation of electric charge is a by-product of Maxwell's equations. Since chemistry is governed by quantum theory and electromagnetism, it is no wonder why charge is conserved in chemical reactions.

1.3.6 Summary

Particles of the same kind are indistinguishable, so we can only count them. N^a, the number of particles of kind a, is an additive and transportable quantity. We denote its density by n^a and its current density by $n^a \boldsymbol{v}^a$. $\boldsymbol{v}^a$ is the average speed of particles of kind a.

Particles disappear or appear in chemical reactions which are described by stoichiometric coefficients ν^{ra}. In each reaction of type r there appear or disappear ν^{ra} particles of kind a, depending on sign. Γ^r is the volumetric reaction rate, the number of chemical reactions of type r per unit volume and per unit time. The volumetric production rate is $\pi(N^a) = \sum_r \Gamma^r \nu^{ra}$.

Mass is conserved in each chemical reaction. Therefore, the mass density ϱ and the mass current density $\varrho \boldsymbol{v}$ obey the continuity equation[7] $\dot{\varrho} + \nabla \cdot \varrho \boldsymbol{v} = 0$. $\boldsymbol{v}$ is the flow velocity of the continuum under investigation.

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[7] A balance equation with vanishing production term is a continuity equation.

We have also shown that the conservation of electric charge is a consequence of Maxwell's equations. The electric charge density ϱ^{e} and the electric current density $\boldsymbol{j}^{\mathrm{e}}$ obey the continuity equation $\dot{\varrho}^{\mathrm{e}} + \nabla \cdot \boldsymbol{j}^{\mathrm{e}} = 0$.

1.4 Convection and Conduction

While matter flows it takes its properties along with it. Therefore there is always a contribution $\varrho(Y)\, v_i$ to the current density $j_i(Y)$. This contribution is termed "convection" because the quantity in question is simply conveyed. Think of a conveyer belt. By definition, mass is transported by convection only, $j_i(M) = \varrho v_i$.

1.4.1 Conduction

However, there may be an additional contribution to the current density,

$$j_i(Y) = \varrho(Y) v_i + J_i(Y). \tag{1.42}$$

This additional current density $J_i(Y)$ describes the conduction of a quantity Y. As said above, there is no conduction of mass. Conduction is caused by interactions between neighboring particles.

The conductive contributions to the particle currents are

$$J_i^a = J_i(N^a) = j_i^a - n^a v_i, \tag{1.43}$$

for which we may write

$$J_i^a = n^a (v_i^a - v_i). \tag{1.44}$$

Particle conduction, or diffusion, takes place if the average velocity of a certain kind of particles $\boldsymbol{v}^a$ differs from the center of mass, or flow velocity $\boldsymbol{v}$. If particles of a certain species move relative to the local center of mass, we speak of diffusion.

The situation is slightly more complicated for the electric charge Q^{e}. The charge density ϱ^{e} may vanish although there are charged particles. In a metal, the mobile electrons and the positive ions of the lattice compensate each other, and the charge density ϱ^{e} vanishes. Nevertheless, there may be an electric current.

The conductive contribution J_i^{e} to the electric current density may be expressed in terms of diffusion current densities:

$$J_i^{\mathrm{e}} = j_i^{\mathrm{e}} - \varrho^{\mathrm{e}} v_i = \sum_a q^a J_i^a. \tag{1.45}$$

1.4.2 Transformation Properties of Currents

As we have just explained, transport is more than convection. There are additional mechanisms like diffusion of particles, electric conduction, mechanical stress, or heat flow.

The decomposition (1.42) of a current density into a convective and a conductive contribution is necessary as well from a formal point of view. We will show now that $\boldsymbol{J}(Y)$ transforms properly as a vector field, but not $\boldsymbol{j}(Y)$. Likewise, $\dot{\varrho}(Y)$ is not a proper scalar field.

Events (what happened where and when) are parameterized by a time coordinate t and three space coordinates[8] x_1, x_2, x_3 referring to an inertial system Σ. The same event has to be parameterized by (t', x'_1, x'_2, x'_3) if another inertial system Σ' is used. The relation is described by a Galilei transformation:

$$t = \tau + t' \text{ and } x_i = a_i + R_{ij} x'_j + u_i t' \text{ with } R_{ij} R_{kj} = \delta_{ik}. \tag{1.46}$$

τ and $\boldsymbol{a}$ describe a time and spatial shift, R a rotation, and $\boldsymbol{u}$ the speed by which Σ moves with respect to Σ'.

A scalar field S is transformed into S' according to

$$S(t, \boldsymbol{x}) = S'(t', \boldsymbol{x}'). \tag{1.47}$$

Densities $\varrho(Y)$, but also volumetric production rates $\pi(Y)$ are scalar fields, because of $\mathrm{d}t' = \mathrm{d}t$ and $\mathrm{d}V' = \mathrm{d}V$.

We conclude that the time derivative of a scalar field is *not* a scalar field because of

$$\partial'_t S' = \partial_t S + u_i \partial_i S. \tag{1.48}$$

Here and in the following text we drop the arguments; primed fields depend on primed coordinates, unprimed fields are to be evaluated at the corresponding unprimed coordinates.

A vector field V_i transforms as

$$V_i(t, \boldsymbol{x}) = R_{ij} V'_j(t', \boldsymbol{x}'). \tag{1.49}$$

The divergence of a vector field is a scalar field:

$$\partial'_i V'_i = R_{ji} \partial'_i V_j = R_{ji} R_{ki} \partial_k V_j = \partial_i V_i. \tag{1.50}$$

Because of

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = R_{ij} \frac{\mathrm{d}x'_j}{\mathrm{d}t'} + u_i \tag{1.51}$$

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[8] We always have a Cartesian system of coordinates in mind.

we find, for an arbitrary scalar field S,

$$S v_i = R_{ij} (S v_j)' + S u_i . \tag{1.52}$$

The divergence of this expression transforms as

$$\partial_i' (S v_i)' = \partial_i (S v_i) - u_i \partial_i S. \tag{1.53}$$

Equations (1.49) and (1.53) say that the sum

$$\partial_t \varrho(Y) + \partial_i \varrho(Y) v_i \tag{1.54}$$

transforms as a scalar field.

We summarize:

- The density $\varrho(Y)$ is a scalar field,
- The production term $\pi(Y)$ is a scalar field,
- The conduction current density $J_i(Y)$ is a vector field.

These transformation properties guarantee that balance equations

$$\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y) \tag{1.55}$$

or

$$\partial_t \varrho(Y) + \partial_i \varrho(Y)\, v_i = -\partial_i J_i(Y) + \pi(Y) \tag{1.56}$$

hold true in all inertial systems.

In the latter version the left hand side, as a sum, transforms as a scalar field just as each of the two contributions on the right hand side.

For further details see section *More on Fields* of Appendix A.

1.4.3 Material Time Derivative

This is the right place to introduce another key notion of continuum physics, the material time derivative D_t . We follow a material point as it flows with the center of mass velocity $\boldsymbol{v}$ and register temporal changes. $f = f(t, \boldsymbol{x})$ is a field, either scalar or a component of a vector field. The material time derivative is defined by

$$\mathrm{D}_t\, f(t, \boldsymbol{x}) = \frac{f(t + \mathrm{d}t, \boldsymbol{x} + \boldsymbol{v}\mathrm{d}t) - f(t, \boldsymbol{x})}{\mathrm{d}t}. \tag{1.57}$$

With

$$f(t + \mathrm{d}t, \boldsymbol{x} + \boldsymbol{v}\mathrm{d}t) = f(t, \boldsymbol{x}) + \mathrm{d}t\, \partial_t\, f(t, \boldsymbol{x}) + \mathrm{d}t\, v_i\, \partial_i\, f(t, \boldsymbol{x}) \tag{1.58}$$

we obtain

$$\mathrm{D}_t = \partial_t + v_i \, \partial_i \tag{1.59}$$

for the material time differentiation operator, or

$$\mathrm{D}_t = \partial_t + \boldsymbol{v} \cdot \nabla. \tag{1.60}$$

1.4.4 Specific Quantities

The density $\varrho(Y)$ is the amount of Y per unit volume. In many situations one better refers to the amount $\sigma(Y)$ of Y per unit mass. We call it a specific quantity. It is defined by

$$\varrho(Y) = \varrho \, \sigma(Y), \tag{1.61}$$

where $\varrho = \varrho(M)$ is the mass density.

We find

$$\mathrm{D}_t \, \varrho = \partial_t \varrho + v_i \, \partial_i \, \varrho = -\varrho \, \partial_i \, v_i \, , \tag{1.62}$$

where we have inserted the mass balance equation. Therefore,

$$\mathrm{D}_t \, \varrho^{-1} = -\varrho^{-2} \, \mathrm{D}_t \, \varrho = \varrho^{-1} \partial_i \, v_i \tag{1.63}$$

holds true. With these preliminaries one can show

$$\varrho \, \mathrm{D}_t \, \sigma(Y) = \varrho(Y) \partial_i \, v_i + \partial_t \varrho(y) + v_i \, \partial_i \, \varrho(Y) = \partial_t \varrho(Y) + \partial_i \, \varrho(Y) v_i \, . \tag{1.64}$$

Equation (1.64) suggests yet another form of the balance equation:

$$\varrho \, \mathrm{D}_t \, \sigma(Y) = -\nabla \cdot \boldsymbol{J}(Y) + \pi(Y). \tag{1.65}$$

The left hand describes a material point which moves with the local center of mass velocity $\boldsymbol{v}$. $\mathrm{D}_t \, \sigma(Y)$ tells how much the specific Y-quantity changes with time, as seen by a co-moving observer. Multiplication with ϱ re-transforms this expression into a density. The left hand side of Eq. (1.65) as well as $\mathrm{D}_t \, \sigma(Y)$ are proper scalar fields.

The right hand side of Eq. (1.65) lists the physical causes for such an increase with time: inflow *by conduction* and production. Note that both terms properly transform as scalars.

By the way, Eq. (1.65), if applied to mass, says that zero equals zero plus zero. The specific mass density is $\sigma(M) = 1$. Clearly, $\varrho \, \mathrm{D}_t \, \sigma(M) = 0$. The mass conduction contribution $\boldsymbol{J}(M)$ vanishes by definition, hence its divergence as well. $\pi(M) = 0$ says that mass cannot be produced or annihilated, but merely redistributed.

1.4.5 Summary

We have presented the generic balance equation in three forms:

- $\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y)$ is the proper choice when establishing partial differential equations for mathematical treatment.
- $\partial_t \varrho(Y) + \partial_i \varrho(Y) v_i = -\partial_i J_i(Y) + \pi(Y)$ separates into a left hand side which is a proper scalar and a right hand side which consists of two contribution each of which transforms properly as a scalar. The conduction current density $\boldsymbol{J}(Y)$ properly transforms as a vector.
- $\varrho\, \mathrm{D}_t\, \sigma(Y) = -\partial_i J_i(Y) + \pi(Y)$ rewrites the left hand side of the former formulation as one term which is easily interpreted from a physics point of view. D_t is the material time differentiation operator and $\sigma(Y)$ the specific Y quantity, i.e., the amount of Y per unit mass.

1.5 Linear and Angular Momentum

Linear momentum is an additive and transportable physical quantity. It is transported not only by convection, but also by conduction. There may be a momentum current even if matter is at rest. This is achieved by electrostatic interactions between neighboring particles. Momentum may also be produced by external forces. We argue why the stress tensor is symmetric. In this slender book we discuss gravitation and electrostatic interaction only. We leave out the third possibility, namely magnetism. The additional formal complications by far outweigh the benefits for the normal reader.

1.5.1 Stress and External Forces

Denote by P_k the kth component of linear momentum $\boldsymbol{P}$. Its density is

$$\varrho(P_k) = \varrho v_k. \tag{1.66}$$

The momentum current density is an object with two indexes, one for the momentum component, the other for the direction of flow. We will write

$$j_i(P_k) = \varrho v_k v_i - T_{ki}, \tag{1.67}$$

where $J_i(P_k) = -T_{ki}$ is the conduction contribution. The negative of it, namely $T_{ki} = T_{ki}(t, \boldsymbol{x})$, denotes the stress tensor field. Upon rotation, each index acquires a rotation matrix, therefore T_{ki} transforms as a tensor of rank 2.

The momentum production rate is the same as external force. The volumetric momentum production rate therefore is a force per unit volume. We here discuss just two such external forces: gravitational and electrostatic. The former is proportional to the mass density, the latter proportional to the electric charge density. We write

$$\pi(P_k) = f_k = \varrho g_k + \varrho^{\mathrm{e}} E_k. \tag{1.68}$$

$\boldsymbol{g}$ is the gravitational force per unit mass and $\boldsymbol{E}$ the electric field strength. In non-inertial systems of reference, terms for fictitious forces must be added, such as the Coriolis force $2\varrho\,\boldsymbol{v} \times \boldsymbol{\Omega}$ per unit volume in a rotating frame.[9]

The momentum balance equation may be written as

$$\varrho\, \mathrm{D}_t\, v_k = \partial_i T_{ki} + f_k. \tag{1.69}$$

We read the left hand side as mass times acceleration per unit volume. The right hand side specifies two causes for this acceleration. One mechanism is by short range interaction (momentum conduction), the other by long range external forces.

1.5.2 Angular Momentum

We denote by L_k the three components of angular momentum $\boldsymbol{L}$. Its density is defined as

$$\varrho(L_k) = \epsilon_{krs} x_r \varrho(P_s), \tag{1.70}$$

where ϵ_{krs} is the totally antisymmetric Levi-Civita symbol.

The corresponding current density is again an object with two indexes,

$$j_i(L_k) = \epsilon_{krs} x_r j_i(P_s). \tag{1.71}$$

Likewise, we write

$$\pi(L_k) = \epsilon_{krs} x_r \pi(L_s) \tag{1.72}$$

for the volumetric angular momentum production rate.

We calculate $\partial_t \varrho(L_k) + \partial_i j_i(L_k) - \pi(L_k)$, which should vanish. The result is

$$\epsilon_{krs} x_r \{\partial_t \varrho(P_k) + \partial_i j_i(P_k) - \pi(P_k)\} + \epsilon_{krs} j_r(P_s). \tag{1.73}$$

Thus, the angular momentum balance equation is fulfilled if $j_r(P_s) = j_s(P_r)$ holds true, and this amounts to

$$T_{rs} = T_{sr}, \tag{1.74}$$

the stress tensor has to be symmetric.

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[9] $\boldsymbol{\Omega}$ describes the direction and the angular velocity of the rotation.

In the above argument we have assumed that angular momentum is orbital angular momentum. This is allowed since we do not consider magnetic fields here. If however magnetic fields come into the play, as in magneto-hydrodynamics, then matter may be magnetically polarized, and a spin angular momentum must be taken into account. In this case, the stress tensor may have an antisymmetric contribution.

1.5.3 Normal and Shear Forces

Let us select a certain material point which flows with velocity $\boldsymbol{v}$. Its acceleration is

$$\varrho\,\mathrm{D}_t\,v_i = \partial_i T_{ki} + f_k, \tag{1.75}$$

as we have argued above. Recall that v_i, T_{ki}, and f_k are fields which depend on time and location. Equation (1.75) holds true at any time t and at any location $\boldsymbol{x}$.

One might think that the stress field itself is of no importance and that just its divergence matters. This, however is not true. As will be discussed in Chap. 2, a construction material can support a maximal stress only. It is therefore worthwhile to look at the stress tensor more closely.

$T_{ki} = T_{ik}$ is real and symmetric, and it can be orthogonally diagonalized. There are three mutually orthogonal unit vectors $\boldsymbol{n}^{(1)}, \boldsymbol{n}^{(2)}, \boldsymbol{n}^{(3)}$ and three eigenvalues $T^{(1)}, T^{(2)}, T^{(3)}$ such that

$$T_{ki}n_i^{(j)} = T^{(j)}n_i^{(j)} \tag{1.76}$$

holds true for $j = 1, 2, 3$. Recall that $T^{(j)}$ as well as $\boldsymbol{n}^{(j)}$ are fields, the may depend on time and on location.

The force exercised by the medium on a surface element $\mathrm{d}\boldsymbol{A} = \mathrm{d}A\,\boldsymbol{n}$ is

$$\mathrm{d}F_k = \mathrm{d}A\,T_{ki}n_i\,. \tag{1.77}$$

This force is directed normal to the surface element if $\mathrm{d}\boldsymbol{F}$ and $\boldsymbol{n}$ are parallel. We speak of a shear force if $\mathrm{d}\boldsymbol{F}$ and $\boldsymbol{n}$ are orthogonal. The normal force component will push the surface element forward, the shear force component tries to put it side-wise.

However, there is no net force on the surface element because the medium draws on the back-side and on the front-size of it with equal, but oppositely directed forces.

If we choose surface elements with normal vectors $\boldsymbol{n}^{(1)}, \boldsymbol{n}^{(2)}, \boldsymbol{n}^{(3)}$, we will not encounter shear forces. Put otherwise, shear forces can always be transformed away, although only locally. However, if we have to solve a real-world problem with one and the same coordinate system, we will encounter shear forces.

By the way, a positive $T^{(j)}$ means tension. The medium on the front-side of the surface elements pulls on it. A negative $T^{(j)}$ indicates pressure. The medium on the front-side of the surface elements pushes on it, it presses. We shall discuss this more closely in the section on *Solid Media*.

1.5.4 Summary

We have introduced the momentum density as mass times velocity per unit volume. This quantity transforms as a vector. The corresponding current density carries two spatial indexes, one for the momentum component and one for the direction of flow. Its conduction contribution is called stress and transforms as a second rank tensor. Without magnetic effects, that is, if angular momentum is orbital angular momentum only and does not have a spin contribution, the stress tensor turns out to be symmetric. Locally, it can be diagonalized orthogonally. This defines three directions such that a corresponding surface element is exposed to normal stress or normal pressure, and no shear forces are encountered. The volumetric momentum production rate is the same as external force per unit volume.

1.6 Energy and the First Law of Thermodynamics

In this section we shall discuss the balance equation for energy. Energy comes in three forms: kinetic, potential, and a rest which is called internal. The balance equations for kinetic energy is a consequence of the momentum balance equation. The potential energy balance equation can easily be established as well. The principle of energy conservation allows to establish the internal energy balance equations. Of particular interest is the volumetric production rate of internal energy, the main result of this section.

1.6.1 Kinetic Energy

The density of kinetic energy E^{k} is one half times mass times velocity squared, per unit volume. As a formula this reads

$$\varrho(E^{\mathrm{k}}) = \frac{1}{2}\varrho v_k v_k. \tag{1.78}$$

$\sigma(E^{\mathrm{k}}) = (1/2)\boldsymbol{v}^2$ is the specific kinetic energy. Its material time derivative is $v_k\, \mathrm{D}_t\, v_k$. Inserting the momentum balance equation as described by Eq. (1.69) yields

$$\varrho\, \mathrm{D}_t\, \sigma(E^{\mathrm{k}}) = v_k\, (\partial_i T_{ki} + f_k\,) = \partial_i v_k T_{ki} - T_{ki} \partial_i v_k + v_k f_k. \tag{1.79}$$

We introduce the symmetric velocity gradient

$$G_{ik} = \frac{\partial_i v_k + \partial_k v_i}{2} \tag{1.80}$$

and may write

$$\pi(E^{\mathrm{k}}) = -G_{ik}T_{ik} + v_k f_k \tag{1.81}$$

as well as

$$j_i(E^{\mathrm{k}}) = -v_k T_{ki}\,. \tag{1.82}$$

Recall that T_{ik} is the stress tensor and f_k the external force per unit volume.

1.6.2 Potential Energy

We now make use of the fact that the electrostatic force as well as the gravitational force have a scalar potential which we denote by ϕ^{e} and ϕ^{g}, respectively:

$$E_k = -\partial_k \phi^{\mathrm{e}} \text{ and } g_k = -\partial_k \phi^{\mathrm{g}}. \tag{1.83}$$

Hence the volumetric production rate of momentum may be written as

$$\pi(P_k) = -\varrho \partial_k \phi^{\mathrm{g}} - \varrho^{\mathrm{e}} \partial_k \phi^{\mathrm{e}}. \tag{1.84}$$

Note that in almost all cases the gravitational potential is just $\phi^{\mathrm{g}}(t, \boldsymbol{x}) = g x_3$ where x_3 denotes height above zero level and $g = 9.81\ \mathrm{m\,s^{-2}}$ is the gravitational acceleration per unit mass at the earth's surface.

For the density oft potential energy E^{p} we write the following expression:

$$\varrho(E^{\mathrm{p}}) = \varrho\phi^{\mathrm{g}} + \varrho^{\mathrm{e}}\phi^{\mathrm{e}}. \tag{1.85}$$

Both potentials are supposed to vary very slowly with time, they are quasi-static. Therefore

$$\partial_t \varrho(E^{\mathrm{p}}) = \phi^{\mathrm{g}} \partial_t \varrho + \phi^{\mathrm{e}} \partial_t \varrho^{\mathrm{e}} = -\phi^{\mathrm{g}} \partial_i j_i(M) - \phi^{\mathrm{e}} \partial_i (Q^{\mathrm{e}}) \tag{1.86}$$

holds true. We rewrite this into a gradient and a rest:

$$\cdots = -\partial_i \phi^{\mathrm{g}} j_i(M) + j_i(M)\partial_i \phi^{\mathrm{g}} - \partial_i \phi^{\mathrm{e}} j_i(Q^{\mathrm{e}}) + j_i(Q^{\mathrm{e}})\partial_i \phi^{\mathrm{e}} \tag{1.87}$$

and conclude

$$j_i(E^{\mathrm{p}}) = \phi^{\mathrm{g}} j_i(M) + \phi^{\mathrm{e}} j_i(Q^{\mathrm{e}}). \tag{1.88}$$

This is a very plausible expression for the potential energy current density.

The remainder is the volumetric potential energy production rate $\pi(E^{\mathrm{p}})$. Because of $j_i(M) = \varrho v_i$ and $j_i(Q^{\mathrm{e}}) = \varrho^{\mathrm{e}} v_i + J_i^{\mathrm{e}}$ we arrive at the following expression:

$$\pi(E^{\mathrm{p}}) = -v_i f_i - J_i^{\mathrm{e}} E_i\,. \tag{1.89}$$

Recall that $\boldsymbol{f}$ is the external force per unit volume, $\boldsymbol{J}^{\mathrm{e}}$ the electric conduction current, and that $\boldsymbol{E}$ denotes the electric field strength.

1.6.3 Internal Energy

There is more than kinetic and potential energy. Material points have a mass, move with average velocity $\boldsymbol{v}$ in a gravitational or electrostatic potential and contribute thereby to the kinetic and to the potential energy. However, material points consist of very many particles, they are large thermodynamic systems. Its constituents have different velocities and interact by short range force. The internal state of a material point gives rise to an energy contribution which we denote by E^{i}.

Note that internal energy is traditionally referred to by U. Therefore we denote by u the *specific* internal energy, the internal energy per unit mass. Hence the density of internal energy is

$$\varrho(E^{\mathrm{i}}) = \varrho u. \tag{1.90}$$

Without mass there will be no internal energy.[10]

Transportation of internal energy by means of conduction is heat conduction. More precisely, the conduction contribution to the internal energy current density is the heat current density which we will denote by $\boldsymbol{J}(E^{\mathrm{i}}) = \boldsymbol{J}^{\mathrm{u}}$. Thus the internal energy current density is

$$j_i(E^{\mathrm{i}}) = \varrho u v_i + J_i^{\mathrm{u}}. \tag{1.91}$$

We know that the sum of kinetic, potential, and internal energy is conserved, $\pi(E^{\mathrm{k}}) + \pi(E^{\mathrm{p}}) + \pi(E^{\mathrm{i}}) = 0$, and conclude

$$\pi(E^{\mathrm{i}}) = T_{ik} G_{ik} + J_i^{\mathrm{e}} E_i. \tag{1.92}$$

We have just shown that the balance equation for internal energy may be written as

$$\varrho \, \mathrm{D}_t \, u = -\partial_i J_i^{\mathrm{u}} + T_{ik} G_{ik} + J_i^{\mathrm{e}} E_i. \tag{1.93}$$

ϱ denotes mass density, u is the specific internal energy and $\boldsymbol{J}^{\mathrm{u}}$ the heat current density. $\boldsymbol{E}$ is the electric field strength and $\boldsymbol{J}^{\mathrm{e}}$ the electric conduction current density. Also recall that T_{ik} denotes the stress tensor and that G_{ik} is the symmetric velocity gradient as defined in Eq. (1.80).

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[10] We do not discuss radiation in this book. Adding a mass independent term for black body radiation of temperature T or any other contribution of energy not bound to mass is an easy exercise.

1.6.4 Digression on Time Reversal

We discuss time reversal in the context of classical mechanics for pedagogical reasons. The results, however, are valid for quantum mechanics as well.

Assume a system of particles with masses m_r and electric charge q_r which, at time t, are located at $\boldsymbol{x}_r(t)$. The particle density is

$$n(t,\boldsymbol{x}) = \sum_r \delta^3(\boldsymbol{x}_r(t) - \boldsymbol{x}), \tag{1.94}$$

the current density

$$\boldsymbol{j}(t,\boldsymbol{x}) = \sum_r \dot{\boldsymbol{x}}_r(t)\, \delta^3(\boldsymbol{x}_r(t) - \boldsymbol{x}). \tag{1.95}$$

Since we study a system with a fixed number of particles, we arrive at

$$\partial_t n + \nabla \cdot \boldsymbol{j} = 0. \tag{1.96}$$

There is no room for chemistry in the framework of classical mechanics.

If there is an electromagnetic field $\boldsymbol{E}$, $\boldsymbol{B}$ the particles suffer accelerations

$$m_r\, \ddot{\boldsymbol{x}}_r(t) = q_r\, \boldsymbol{E}(t,\boldsymbol{x}_r(t)) + q_r\, \dot{\boldsymbol{x}}_r(t) \times \boldsymbol{B}(t,\boldsymbol{x}_r(t)). \tag{1.97}$$

On the other hand, the electromagnetic field is generated by the charged particles. The electric charge density is

$$\varrho^{\mathrm{e}}(t,\boldsymbol{x}) = \sum_r q_r\, \delta^3(\boldsymbol{x}_r(t) - \boldsymbol{x}), \tag{1.98}$$

the electric current density is given by

$$\boldsymbol{j}^{\mathrm{e}}(t,\boldsymbol{x}) = \sum_r q_r\, \dot{\boldsymbol{x}}_r(t)\, \delta^3(\boldsymbol{x}_r(t) - \boldsymbol{x}). \tag{1.99}$$

Charge conservation

$$\partial_t \varrho^{\mathrm{e}} + \nabla \cdot \boldsymbol{j}^{\mathrm{e}} = 0 \tag{1.100}$$

is a trivial consequence of these definitions.

The electromagnetic field is generated according to Maxwell's equations:

$$\epsilon_0 \nabla \cdot \boldsymbol{E} = \varrho^{\mathrm{e}}, \tag{1.101}$$

$$\nabla \cdot \boldsymbol{B} = 0, \tag{1.102}$$

$$-\epsilon_0 \partial_t \boldsymbol{E} + \frac{1}{\mu_0} \nabla \times \boldsymbol{B} = \boldsymbol{j}^{\mathrm{e}}, \tag{1.103}$$

and

$$\partial_t \boldsymbol{B} + \nabla \times \boldsymbol{E} = 0. \tag{1.104}$$

The constants ϵ_0 and μ_0 are the vacuum permittivity and permeability, respectively. Their values depend on the system of units.

Time reversal T means to replace trajectories $t \to \boldsymbol{x}(t)$ by time reversed trajectories, namely $t \to \boldsymbol{x}'(t) = \boldsymbol{x}(-t)$. With this we deduce the following field equations[11]:

$$n^\star(t, \boldsymbol{x}) = n(-t, \boldsymbol{x}) \text{ and } \boldsymbol{j}^\star(t, \boldsymbol{x}) = -\boldsymbol{j}(-t, \boldsymbol{x}) \tag{1.105}$$

as well as

$$\varrho^{\mathrm{e}\star}(t, \boldsymbol{x}) = \varrho^{\mathrm{e}}(-t, \boldsymbol{x}) \text{ and } \boldsymbol{j}^{\mathrm{e}\star}(t, \boldsymbol{x}) = -\boldsymbol{j}^{\mathrm{e}}(-t, \boldsymbol{x}). \tag{1.106}$$

Maxwell's equations are compatible with time reversal if

$$\boldsymbol{E}^\star(t, \boldsymbol{x}) = \boldsymbol{E}(-t, \boldsymbol{x}) \text{ and } \boldsymbol{B}^\star(t, \boldsymbol{x}) = -\boldsymbol{B}(-t, \boldsymbol{x}) \tag{1.107}$$

are fulfilled. Compatible means that the time reversed fields, as generated by the time reversed electric charge and current density, are solutions of Maxwell's equations as well.

The Lorentz formula (1.97) for the action of the electromagnetic field on a charged particle is compatible with time reversal as well. On the one hand, $m_r \ddot{\boldsymbol{x}}_r{}^\star(t) = m_r \ddot{\boldsymbol{x}}_r(-t)$. On the other hand, $q_r \boldsymbol{E}(t, \boldsymbol{x}_r{}^\star(t))$ is the same as $q_r \boldsymbol{E}(-t, \boldsymbol{x}_r(-t))$. The same holds true for the second contribution to the Lorentz force since velocity and magnetic induction acquire a minus sign upon time reversal.

1.6.5 First Law of Thermodynamics

The first law of thermodynamic is a statement about the change of internal energy in the course of time, as described by Eq. (1.93). The increase in internal energy, as measured by a co-moving observer, is caused by a net inflow of internal energy by conduction and by two more terms which are proportional to the velocity gradient G_{ij} and to the electric field strength $\boldsymbol{E}$. The factor in front is the stress tensor T_{ij} and the electric conduction current $\boldsymbol{J}^{\mathrm{e}}$, respectively. See Fig. 1.1 for a sketch.

These factors are conduction current densities of momentum and of electric charge. We should split each of them into two contributions, namely into $T_{ik} = T'_{ik} + T''_{ik}$ and $J^{\mathrm{e}}_i = J^{\mathrm{e}\,\prime}_i + J^{\mathrm{e}\,\prime\prime}_i$. The primed contribution behaves normally with respect to time reversal, as explained above. However, since thermodynamics does not deal with small, isolated systems, but takes interactions with the environment into account, there may be abnormal contributions to currents. Upon time reversal they do not acquire a minus, but a plus sign. The doubly primed currents describe

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[11] A star denotes the time reversed quantity, in this context.

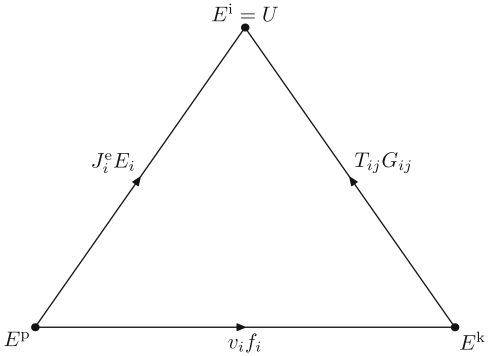

Fig. 1.1 Volumetric production rates for kinetic, potential, and internal energy. If the *arrow* points towards an energy contribution, the corresponding expression enters the balance equation with a *plus sign*

inelastic, or dissipative effects while the single primed currents stand for reversible, or elastic processes.

The first law of thermodynamics thus reads

$$\varrho \, \mathrm{D}_t \, u = T'_{ik} G_{ik} + J^{\mathrm{e}\,\prime}_i E_i - \partial_i J^{\mathrm{u}}_i + T''_{ik} G_{ik} + J^{\mathrm{e}\,\prime\prime}_i E_i \,. \tag{1.108}$$

The first two terms are from elastic contributions and are associated with work. $T'_{ik} G_{ik}$ causes an increase in internal energy because of compression or deformation of matter, as we shall explain later in detail. $J^{\mathrm{e}\,\prime}_i E_i$ describes the increase of internal energy because of dielectric polarization.

The remaining three terms in Eq. (1.108) are associated with heat. This denomination is evident for $\partial_i J^{\mathrm{u}}_i$, the net outflow of internal energy. If the internal energy of a material point increases, its temperature will rise.[12]

The fourth term $T''_{ik} G_{ik}$ describes the generation of internal energy by friction which is irreversible. Older texts sometimes speak of friction heat.

The fifth contribution to Eq. (1.108) is called Joule's heat, the conversion of electric field energy into internal energy.

Multiplying Eq. (1.108) by dt and by dV yields

$$\mathrm{d}U = \mathrm{d}W + \mathrm{d}Q \,, \tag{1.109}$$

an abbreviated version of the first law of thermodynamics. dU says that there is an additive and transportable quantity U, the internal energy. It may change because of two mechanisms, reversible or not. The reversible part is dW, or work, the irreversible contribution dQ is heat.

dW and dQ denote infinitesimal changes. There are no additive and transportable quantities W (for work) or Q (for heat). If you think of a brick, you may speak of its kinetic energy, its potential energy, and of its internal energy. The internal energy

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[12] *Heat* and *hot* are related words in ordinary English, just as *Wärme* and *warm* in everyday German, or *calor* and *calido* in Spanish.

content, however, may not be divided into work or heat. The notions of work or heat refer to different mechanisms of energy transport.

With

$$\mathrm{d}U = \mathrm{d}t\mathrm{d}V\,\varrho\,\mathrm{D}_t\,u, \tag{1.110}$$

$$\mathrm{d}W = \mathrm{d}t\mathrm{d}V\,T'_{ik}G_{ik} + \mathrm{d}t\mathrm{d}V\,J^{\mathrm{e}\,\prime}_i E_i, \tag{1.111}$$

and

$$\mathrm{d}Q = -\mathrm{d}t\mathrm{d}V\,\partial_i J^{\mathrm{u}}_i + \mathrm{d}t\mathrm{d}V\,T''_{ik}G_{ik} + \mathrm{d}t\mathrm{d}V\,J^{\mathrm{e}\,\prime\prime}_i E_i \tag{1.112}$$

we are less general, but much more precise. We clearly say what is the change of internal energy and identify its causes. Reversible and irreversible. Elastic deformation or electric polarization, friction or Joule's heat. And heat conduction.

In the absence of external magnetic fields *this is all.*

By the way, the volumetric production rate for internal energy does not contain a contribution due to chemistry. Chemical reactions, as described by their volumetric reaction rates Γ^r, do not show up. They will appear in the expression of entropy production, which is the topic of the next section.

1.6.6 Summary

Energy is either kinetic, or potential, or internal. The kinetic and potential energy balance equations are easily derived from the momentum balance equations. The internal energy of material points may change because of five effects which are classified as work and heat. Work is achieved by the reversible compression or deformation of matter or by electric polarization. The change of internal energy by irreversible processes (heat) comes from an inflow of internal energy by conduction, by friction, or by the irreversible transformation of electromagnetic field energy into internal energy which is known as Joule's heat. A digression on time reversion intends to elucidate the difference between normal and abnormal behavior of currents, or elastic and inelastic (i.e., dissipative) effects.

1.7 Entropy and the Second Law of Thermodynamics

This section is about the very heart of continuum physics. We will cast into equations the idea that material points are tiny as seen by an engineer and huge in terms of thermodynamics. Processes, such as the combustion of an air-fuel mixture in a jet engine, are slow on a micro-physics scale, so that we may assume that each material point is always very close to thermal equilibrium. However, the parameters which govern this local thermal equilibrium are fields, they change with time and depend on location. Although matter is locally in thermodynamic equilibrium, globally it may be far away from it.

1.7.1 Thermodynamic Equilibrium

Thermodynamic equilibrium is described by the free energy

$$F = F(T, \lambda_1, \lambda_2, \dots, N^1, N^2, \dots). \tag{1.113}$$

T denotes the absolute temperature, $\lambda_1, \lambda_2 \dots$ are external parameters, and N^a denotes the number of particles of species a. The partial derivatives of the free energy can be read off from

$$\mathrm{d}F = -S\mathrm{d}T + \mathrm{d}W + \sum_a \mu^a \mathrm{d}N^a, \tag{1.114}$$

where S is the entropy of the system,

$$\mathrm{d}W = -\sum_i \Lambda_i \, \mathrm{d}\lambda_i \quad \text{with} \quad \Lambda_i = -\frac{\partial F}{\partial \lambda_i} \tag{1.115}$$

is called work, and the μ^a are chemical potentials. The partial derivatives Λ_i are generalized forces.

We prefer to invoke the internal energy U which is defined by $U = F + TS$. Its dependencies on thermodynamic variables and its partial derivatives are to be read off from

$$\mathrm{d}U = T\mathrm{d}S + \mathrm{d}W + \sum_a \mu^a \mathrm{d}N^a. \tag{1.116}$$

Let us now translate this into the language of continuum theory.

1.7.2 Balance Equation for Entropy

We select a material point with constant mass M. Its volume $V = V(t, \boldsymbol{x})$ may change and consequently the density $\varrho(t, \boldsymbol{x}) = M / V(t, \boldsymbol{x})$.

Let us denote by $s = \sigma(S)$ the specific entropy so that we may write

$$\mathrm{d}S = \mathrm{d}tM \, \mathrm{D}_t \, s = \mathrm{d}t \; V\varrho \, \mathrm{D}_t \, s. \tag{1.117}$$

A co-moving observer measures the change of entropy per unit mass. The result is multiplied by the time span $\mathrm{d}t$ and the mass $V\varrho$ the result of which is the change of entropy.

The change of internal energy $\mathrm{d}U = \mathrm{d}t \; V \, \mathrm{D}_t \, u$ has been worked out before:

$$\mathrm{d}U = \mathrm{d}t \; V \, \{-\partial_i J^{\mathrm{u}}_i + T'_{ik} G_{ik} + T''_{ik} G_{ik} + J^{\mathrm{e}}_i{}' E_i + J^{\mathrm{e}}_i{}'' E_i \}. \tag{1.118}$$

Recall that $\boldsymbol{J}^{\mathrm{u}}$ is the heat current, $G_{ik} = (\partial_i v_k + \partial_k v_i)/2$ the symmetric velocity gradient, T_{ik} the stress tensor and $\boldsymbol{J}^{\mathrm{e}}$ the electric conduction current. The latter two are split into elastic and dissipative contributions as indicated by a prime or a double prime.

The reversible contributions are associated with work:

$$\mathrm{d}W = \mathrm{d}t\, V\, \{T'_{ik} G_{ik} + J^{\mathrm{e}\,\prime}_i E_i\}. \tag{1.119}$$

Changes of chemical composition are expressed by

$$\mathrm{d}N^a = M \mathrm{d}t\, \mathrm{D}_t \frac{n^a}{\varrho} = \mathrm{d}t\, V\, \{-\partial_i J^a_i + \sum_r \Gamma^r \nu^{ra}\}. \tag{1.120}$$

Recall that $\boldsymbol{J}^a$ is the diffusion current density for particles of species a. The ν^{ra} are stoichiometric coefficients for the chemical reaction labeled by r, and Γ^r is the number of such reactions per unit time and volume. We have discussed this in the section on *Particle numbers, mass, and electric charge*.

We now insert Eqs. (1.117)–(1.120) into Eq. (1.116) and obtain

$$T\varrho\, \mathrm{D}_t\, s = -\partial_i J^u_i + T''_{ik} G_i k + J^{\mathrm{e}\,\prime\prime}_i + \sum_a \mu^a \partial_i J^a_i + \sum_r \Gamma^{ra} A^r. \tag{1.121}$$

The symbols

$$A^r = -\sum_a \nu^{ra} \mu^a \tag{1.122}$$

stand for the chemical affinity of a reaction of type r.

Dividing Eq. (1.121) by the absolute temperature T we obtain the balance equation $\partial_t \varrho(S) + \partial_i j_i(S) = \pi(S)$ for entropy.

The entropy current density is easily worked out,

$$\boldsymbol{j}(S) = \varrho s \boldsymbol{v} + \frac{1}{T} \boldsymbol{j}^{\mathrm{u}} - \sum_a \frac{\mu^a}{T} \boldsymbol{J}^a. \tag{1.123}$$

Entropy is transported by the flow of matter, or convection. This is the first term. Entropy also flows if there is a heat current. The heat current is weighted by the inverse temperature. The smaller the temperature, the more entropy is conducted. The third term on the right hand side of Eq. (1.123) says that entropy is also transported by diffusion. A diffusion current is weighted by the ratio of negative chemical potential and temperature.

The volumetric production rate of entropy will be discussed in the following subsection. It is more than an expression of fields which we have introduced before. The second law of thermodynamics states that it cannot be negative.

1.7.3 Second Law of Thermodynamics

When rewriting Eq. (1.121) into a balance equation for entropy, we have selected all terms which are divergences. The corresponding current is Eq. (1.123). The remainder is $\pi(S)$, namely the entropy production rate per unit volume. It reads

$$\pi(S) = \pi^{\text{hc}} + \pi^{\text{df}} + \pi^{\text{fr}} + \pi^{\text{jh}} + \pi^{\text{ch}}. \tag{1.124}$$

It consists of five, and only five terms.[13]

$$\pi^{\text{hc}} = J_i^{\text{u}}\, \partial_i \frac{1}{T} \tag{1.125}$$

describes entropy production because of heat conduction (hc). Recall that $\boldsymbol{J}^{\text{u}}$ is the heat current density. Entropy is produced only if the temperature has a non-vanishing gradient.

$$\pi^{\text{df}} = -\sum_a J_i^a\, \partial_i \frac{\mu^a}{T} \tag{1.126}$$

says that diffusion (df) is accompanied by an increase of entropy. $\boldsymbol{J}^a$ is the diffusion current of particles of species a. Entropy is produces only if the chemical potential μ^a divided by the temperature T has a non-vanishing gradient.

The third contribution is related to friction (fr). G_{ik} is a measure of how much the velocity component v_k changes with respect to direction i, or how much the velocity component v_i changes with respect to direction k. Different layers flow with different velocities, and this produces friction by short range forces between neighboring layers. Friction contributes to the volumetric production of entropy by the term

$$\pi^{\text{fr}} = \frac{1}{T}\, T''_{ik}\, G_{ik} = \frac{1}{T}\, T''_{ik}\, \frac{\partial_i v_k + \partial_k v_i}{2}. \tag{1.127}$$

Note that it is the dissipative contribution to the stress tensor which multiplies the velocity gradient.

The fourth term describes the contribution of Joule's heat to entropy production:

$$\pi^{\text{jh}} = \frac{1}{T}\, J_i^{\text{e}\,\prime\prime} \partial_i \phi^{\text{e}}. \tag{1.128}$$

Recall that we here discuss only quasi-stationary electric fields which have a potential, $\boldsymbol{E} = -\nabla\phi^{\text{e}}$.

Entropy is also produced if chemical reactions take place, so

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[13] If magnetic effects are ignored.

$$\pi^{\mathrm{ch}} = \frac{1}{T} \sum_r \Gamma^r A^r. \tag{1.129}$$

The larger the chemical affinity for reaction r, and the more reactions take place, the more entropy will be produced.

The second law of thermodynamics assures

$$\pi(S) \geq 0. \tag{1.130}$$

All contributions have the same structure. They are products of a dissipative current which is multiplied by an expression which would vanish in thermodynamic equilibrium.

If matter is in a global equilibrium state then the temperature T, the chemical potentials μ^a, the flow velocity $\boldsymbol{v}$ and the electric potential ϕ^{e} will be constant and all chemical activities vanish. There is no entropy production if the system is in thermodynamic equilibrium.

Likewise, if there are no heat or diffusion currents, if there is no dissipative stress (super-fluidity) and no dissipative electric current (superconductivity), and if there are no chemical reactions: in this case no entropy is produced either.

1.7.4 Summary

A continuum is locally in thermodynamic equilibrium, but not necessarily globally. Hence, each material point may be characterized by its temperature and by its chemical potentials. These thermodynamic quantities, however, are fields, they will change from location to location and in the course of time. The material points undergo reversible processes. From this we derive expressions for the entropy current density $\boldsymbol{j}(S)$ and for the volumetric entropy production rate $\pi(S)$. The latter consists of five, and only five contributions, for heat conduction, diffusion, friction, Joule's heat, and chemical activity. None of these terms can be negative, according to the second law of thermodynamics.

Chapter 2
Material Equations

In the preceding chapter of this book on *Continuum Physics* we have discussed the notion of material points. They are infinitely small from a macroscopic point of view and infinitely large from a microscopic point of view. Just think of the temperature field $T = T(t, \boldsymbol{x})$. The material point at location $\boldsymbol{x}$ at time t is large enough for obeying the rules of infinitely large systems, such as the ideal gas law, for example. On the other hand, it is small enough so that it approaches thermodynamic equilibrium practically immediately. The state of the material point is always an equilibrium, or Gibbs state which is characterized by parameters such as temperature or chemical potentials. Hence $T = T(t, \boldsymbol{x})$ is defined locally, but may change from location to location and within the course of time.

From a microscopic point of view, a material point is so large that it is rather clear whether a particle is inside or outside of it. Those particles which are partly inside and partly outside form a vanishing minority. Hence, densities are well defined. The same applies to current densities and to volumetric production rates. If something inside a material point increases, it must have been migrated from outside to inside, or it has been produced there. This reasoning is formulated as a balance equation.

We have discussed balance equations for particles of a certain species, for matter and electric charge. If these particles move, they carry their properties with them. These properties, however, may be conveyed as well by interaction. The balance equations for linear momentum and for kinetic, potential, and internal energy are examples. The notion of internal energy, however, alludes to the fact that material points are more than small pieces of mass and charge. Poetically speaking, they have their own life. In particular, they carry energy which is termed internal.

If, moreover, the material point is in thermodynamic equilibrium with its environment, and keeps to be so, it undergoes a reversible process. In the section on entropy we have worked out expressions for the entropy current density and the volumetric entropy production rate. The latter expression, consisting of five terms and should never be negative. This is the essence of the Second law of thermodynamics.

Up to now there is just a continuum. All balance equations must be fulfilled. However, there are far too many fields and too few equations for them. In order to arrive at solutions for a specific problem we have to specify the material at hand.

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By specifying particular material equations we describe different fields of applications, such as hydrodynamics, aerodynamics, elastodynamics, heat transport, diffusion, charge transport, thermo-electrical effects, or optics. We refrain from discussing material equation for chemistry[1] because this is a book on the physics of continuous media, not on chemistry.

2.1 Fluid Media

A fluid medium[2] cannot support shear forces. More precisely, the reversible part of the stress tensor must be such that $\mathrm{d}F_i = T'_{ij}\mathrm{d}A_j$ is proportional to $\mathrm{d}A_i$. There is no perpendicular component, no shear force. Recall that we denote by $\mathrm{d}\boldsymbol{A}$ an infinitesimal area element and by $\mathrm{d}\boldsymbol{F}$ the force exercised on it.

Therefore, a fluid medium has to be described by the following material equation:

$$T'_{ij} = -\delta_{ij}\, p, \tag{2.1}$$

where $p = p(t, \boldsymbol{x})$ is the pressure field. The minus sign is a convention. Normally, pressure is positive, such that the medium on the front of $\mathrm{d}\boldsymbol{A}$ tries to repel the surface element. The medium on the backside exercises the same, but oppositely directed force.

Water and air may serve as prototypes of fluid media. Under ordinary conditions, water is a fluid proper, i.e., a liquid. Air under normal conditions behaves, to a very good approximation, as an ideal gas. “Normal” in this context means “as encountered in nature”.

In the following we will discuss these idealizations in some length, while we just touch how to describe non-ideal gases and not-Newtonian fluids.

The momentum balance equation (1.69) for a fluid reads

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\partial_k p + f_k + \partial_i T''_{ik}. \tag{2.2}$$

The left hand side of this equation is simply $\varrho\, \mathrm{D}_t\, v_k$, i.e., mass times acceleration per unit volume, as felt by a co-moving observer. On the right hand side we find three terms which describe the cause of acceleration: pressure gradient, external forces, and friction.

2.1.1 Incompressible Fluids

Water and many oils are practically incompressible media. Their mass density does only weakly depend on pressure and on temperature. $\varrho(t, \boldsymbol{x}) =$ const. is a good approximation within a reasonable pressure and temperature interval.

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[1] The article on *Reaction and diffusion* is an exception

[2] As contrasted with a solid medium.

Because of $\partial_t \varrho + \partial_i \varrho v_i = 0$ we conclude

$$\partial_i v_i = 0. \tag{2.3}$$

The velocity field of an incompressible fluid is divergence-free. Solutions of the momentum balance equation (2.2) must additionally fulfill Eq. (2.3).

We mention in passing that a divergence-free field may be represented as the curl of a vector potential, $\boldsymbol{v} = \boldsymbol{\nabla} \times \boldsymbol{A}$. One can rewrite the momentum balance equation (2.2) in terms of a vector potential $\boldsymbol{A}$. A solution then automatically yields a divergence-free vector field. There is, however, a serious drawback. There are many vector potentials for one and the same velocity field.

2.1.2 Ideal Gas

If the specific volume of a gas is sufficiently large, it behaves as if there were no interactions between its particles, it behaves ideally.

The partial pressure of particles of species a is given by

$$p_a = k_{\mathrm{B}} T \, n_a, \tag{2.4}$$

where n_a denotes particle density, and T is the absolute temperature. The partial pressures of a mixture of ideal gases add up,

$$p = \sum_a k_{\mathrm{B}} T \, n_a. \tag{2.5}$$

We define the molar fractions x_a by

$$x_a = \frac{n_a}{n} \text{ where } n = \sum_a n_a. \tag{2.6}$$

n is the total number of particles per unit volume, and x_a is the percentage of particles of species a. Note that $\sum_a x_a = 1$.

The mass density is

$$\varrho = \sum_a m_a n_a, \tag{2.7}$$

where m_a is the mass of a particle of species a. We may write

$$\varrho = \sum_a m_a x_a \, n = mn \text{ with } m = \sum_a x_a m_a. \tag{2.8}$$

m is the average particle mass with respect to a composition $x_1, x_2, \dots$. The ideal gas law (2.5) may thus be rewritten as

$$p = \frac{\varrho}{m} k_{\mathrm{B}} T. \tag{2.9}$$

The latter form (2.9) is a substantial simplification if the composition of the ideal gas mixture remains constant. Then, m is a constant, and we may express the pressure field in terms of temperature and mass density. Air within the troposphere[3] is an example.

There is still something to be repaired. Boltzmann's constant k_{B} and the average molecular mass m hint at micro-physics. We multiply both quantities by Avogadro's number N_{A}. Recall that the amount of N_{A} particles is a mole[4] in terms of chemistry. $R = N_{\mathrm{A}} k_{\mathrm{B}}$ is the universal gas constant,[5] $M = N_{\mathrm{A}} m$ the average molar mass. With this Eq. (2.9) reads

$$p = \frac{\varrho}{M} R T. \tag{2.10}$$

R is the universal gas constant. Pressure p, temperature T and mass density ϱ are fields. For most problems the average molar mass M is a constant as well.[6]

2.1.3 Newtonian Fluid Medium

The dissipative contribution T''_{ik} must be a symmetric tensor which behaves nonstandard under time reversal. It describes friction. There is no friction if neighboring material points travel with the same velocity. Hence, the dissipative contribution to the stress tensor will depend on velocity gradients. A Newtonian fluid is characterized by a linear dependency which is a very good approximation for many liquids and gases, such as water and air.

The symmetric velocity gradient G_{ik} may be split into a trace part $\delta_{ik} G_{jj}$ and a traceless rest. Both are linear in velocity gradients, behave as second order rank tensors and transform odd under time reversal. Hence we write

$$T''_{ik} = \eta^{\mathrm{b}} \delta_{ik} G_{jj} + 2\eta^{\mathrm{s}} \left\{ G_{ik} - \frac{1}{3} \delta_{ik} G_{jj} \right\}. \tag{2.11}$$

η^{b} is the *b*ulk (or volume) viscosity while η^{s} denotes the *s*hear viscosity. Only the latter comes into play if we investigate incompressible fluids.[7]

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[3] The region which is afflicted by weather phenomena, roughly the first 15 km. It contains 75% of the air mass and more than 98% of water vapor.

[4] One mole of the isotope ^{12}C has a mass of exactly 0.012 kg, by definition.

[5] $R = 8.314\ \mathrm{J\,K^{-1}\,mol^{-1}}$.

[6] 0.02897 $\mathrm{kg\,mol^{-1}}$ for dry air.

[7] Recall $G_{jj} = \partial_j v_j$.

The divergence $\partial_i T''_{ik}$ of (2.11) is

$$\eta^{\mathrm{s}} \Delta v_k + \eta^{\mathrm{s}} \partial_k \partial_j v_j - \frac{2\eta^{\mathrm{s}}}{3} \partial_k \partial_j v_j + \eta^{\mathrm{b}} \partial_k \partial_j v_j . \tag{2.12}$$

Therefore, the momentum balance equation for a Newtonian fluid medium reads

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\partial_k p + f_k + \eta^{\mathrm{s}} \Delta v_k + \{\frac{\eta^{\mathrm{s}}}{3} + \eta^{\mathrm{b}}\} \partial_k \partial_j v_j . \tag{2.13}$$

We should work out the consequences of the second law of thermodynamics. The volumetric entropy production rate caused by friction is

$$\pi^{\mathrm{fr}} = \frac{1}{T} T''_{ik} G_{ik} = \frac{\eta^{\mathrm{b}} - 2\eta^{\mathrm{s}}/3}{T} (G_{jj})^2 + \frac{2\eta^{\mathrm{s}}}{T} G_{ik} G_{ik} . \tag{2.14}$$

T denotes absolute temperature which is always positive.

If we choose a divergence-free velocity field, $\pi^{\mathrm{fr}} \geq 0$ can only be guaranteed if the shear viscosity vanishes or is positive,

$$\eta^{\mathrm{s}} \geq 0. \tag{2.15}$$

If we insert a velocity field $\boldsymbol{v} = \gamma \boldsymbol{x}$, Eq. (2.14) yields $9(\eta^{\mathrm{b}} - 2\eta^{\mathrm{s}}/3)\gamma^2 + 6\eta^{\mathrm{s}}\gamma^2$, divided by T, hence $9\eta^{\mathrm{b}}\gamma^2/T$. The second law of thermodynamics hence demands

$$\eta^{\mathrm{b}} \geq 0. \tag{2.16}$$

2.1.4 Hydrodynamics

To a very good approximation, water is incompressible and behaves as a Newtonian fluid. Thus we have to specialize Eq. (2.13) to $\partial_j v_j = 0$.

The momentum balance equation for an incompressible Newtonian fluid reads

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\partial_k p + f_k + \eta \, \Delta v_k . \tag{2.17}$$

This is the famous Navier-Stokes equation which governs the field of hydrodynamics. ϱ, the mass density is considered to be constant. $\boldsymbol{v}$ denotes the velocity field, p is the pressure field, $\boldsymbol{f}$ are external forces per unit volume. $\eta = \eta^{\mathrm{s}}$ is the (shear) viscosity of the fluid. Note that only divergence-free velocity fields are admissible.

The term $\varrho v_i \partial_i v_k$ is quadratic in the velocity field and poses problems for finding analytic or numerical solutions. It should be compared with the friction term $\eta \Delta v_k$. If v is a typical velocity of a problem and ℓ a typical length, then

$$\mathtt{Re} = \frac{\varrho v \ell}{\eta} \tag{2.18}$$

is an estimate of the ratio of inertial to frictional forces. `Re` is called Reynold's number, it is dimensionless.

A small Reynold number means that friction is dominant, the fluid will flow in smooth layers that glide one over the other. One also speaks of laminar flow. A large Reynold number predicts turbulence. $\mathtt{Re} \approx 10^4$ is a very rough guess for the onset of turbulence.

Even if the quadratic-in-velocity term $\varrho v_i \partial_i v_k$ vanishes because of symmetry reasons, the corresponding solution might be unstable if the Reynold number of the problem is too big.

2.1.5 Aerodynamics

The basic material equations for aerodynamics are Newton's expression (2.11) for internal friction and the ideal gas law (2.10) with a constant molar mass M. Even with these simplifications, and only if the mechanical aspect is considered, the problem at hand is already formidable.

The mass density will not be constant, therefore

$$\partial_t \varrho + \partial_i \varrho v_i = 0 \tag{2.19}$$

must hold. Mass density ϱ and the speed $\boldsymbol{v}$ of flow are interlinked.

The momentum balance equation, with the ideal gas law, reads

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\frac{R}{M} \partial_k \frac{\varrho}{T} + f_k + \eta^{\mathrm{s}} \Delta v_k + \left\{ \frac{\eta^{\mathrm{s}}}{3} + \eta^{\mathrm{b}} \right\} \partial_k \partial_j v_j . \tag{2.20}$$

Another field enters the stage, namely temperature T. Often heat conduction in gases may be neglected; then the flow is adiabatic. For a gas of diatomic molecules the following state equation then holds:

$$\frac{T}{T_0} = \left\{ \frac{\varrho}{\varrho_0} \right\}^{2/5} . \tag{2.21}$$

(T_0, ϱ_0) is a reference point.

Altogether we have five fields: mass density ϱ, the three velocity components v_k, and temperature T. Equations (2.19)–(2.21) are likewise five partial differential equations. They are intimately coupled.

Note that the shear viscosity η^{s} as well as the bulk viscosity η^{b} will depend on mass density and on temperature, they may become fields. Additional material equations $\eta^{\mathrm{s}} = \eta^{\mathrm{s}}(\varrho, T)$ and $\eta^{\mathrm{b}} = \eta^{\mathrm{b}}(\varrho, T)$ have to be specified, if necessary.

Aerodynamics is a vast field. Just think of airplane or automotive engineering, meteorology and climate models, or such simple things as Bernoulli's law. We have just scratched the surface. Non-ideal gases, non-Newtonian friction, non-adiabatic flows, chemical reactions such as combustion in a jet engine, and many, many more effects must be taken into account in real-world problems. It is out of the scope of this book to go into details.

A non-ideal gas is characterized by a power series

$$p = \frac{RT}{M}\{\varrho + B_2\varrho^2 + \cdots\}, \tag{2.22}$$

the so called virial expansion. The coefficients B_2, B_3 and so forth depend on temperature, they can be calculated if the interaction potential between the molecules is known.[8] It is a fortunate accident that $B_2 = B_2(T)$ for air nearly vanishes at room temperature. Carbon dioxide behaves differently. Similar considerations apply for the osmotic pressure of solvents.

Non-Newtonian friction is, well, non Newtonian. There are many causes for a deviation. The relationship between the dissipative part of the stress tensor and the velocity gradient may be linear, but retarded. This is the case for glasses which behave as elastic solids for short times and as liquids in the long run. Or T''_{ij} depends other than linear on the velocity gradient G_{ij}. A non-laminar air flow may serve as an example.

2.1.6 Summary

A fluid medium, gas or liquid, cannot support static, or reversible shear forces. It is characterized by a pressure field. Very simple, but realistic idealizations are incompressible fluids and ideal gases. We have studied in some detail the concept of a Newtonian fluid medium the internal frictional forces of which are linear functions of the velocity gradients. The dynamics of water, or hydrodynamics, is governed by the Navier-Stokes equation. The Reynold number decides whether the flow is laminar or turbulent. Aerodynamics, the dynamics of air, is even more complicated because temperature comes into the game.

2.2 Solid Media

In contrast with a fluid medium, a solid may support static shear forces. That makes it a solid: it requires strong forces to deform it. Even the elastic part T'_{ik} may have non-diagonal entries. If the solid is relaxed, i.e., if no external forces are exercised, there will be no stress. If, however, the solid medium suffers strain, there will be stress. We shall formulate the idea that, to a first approximation, stress and strain are proportional which is known as Hooke's law. Before we must explain the notion of strain.

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[8] By the way, one speaks of *the* ideal gas because $B_1 = 1$ holds true for all kinds of molecules.

2.2.1 Strain

Think of a material point at a certain location $\boldsymbol{x}$. These are the coordinates with respect to a Cartesian coordinate system if the medium is relaxed. "Relaxed" means that no forces are present, neither volume forces nor forces upon the boundary of the medium. We speak of the relaxed state of the solid medium.

If, however, such forces act on the medium, if it is deformed, the material points of the continuum will be displaced. The material point, formerly at $\boldsymbol{x}$, will now be at $\bar{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{u}$. $\boldsymbol{u} = \boldsymbol{u}(t, \boldsymbol{x})$ is the displacement field, it describes the displacement, at time t, of a point which was situated at $\boldsymbol{x}$ before the displacement, when the medium was relaxed.

Two neighboring points at $\boldsymbol{x}$ and $\boldsymbol{x} + \mathrm{d}\boldsymbol{x}$ in the relaxed state will be found at $\bar{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{u}(t, \boldsymbol{x})$ and $\bar{\boldsymbol{x}} + \mathrm{d}\bar{\boldsymbol{x}} = \boldsymbol{x} + \mathrm{d}\boldsymbol{x} + \boldsymbol{u}(t, \boldsymbol{x} + \mathrm{d}\boldsymbol{x})$ in the stressed state. In the relaxed state, before deformation, their distance was $\mathrm{d}s$ where

$$\mathrm{d}s^2 = \mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2 = \delta_{ik} \mathrm{d}x_i \mathrm{d}x_k . \tag{2.23}$$

With

$$\mathrm{d}\bar{x}_i = \mathrm{d}x_i + \mathrm{d}x_j \, \partial_j u_i(t, \boldsymbol{x}) \tag{2.24}$$

we arrive at

$$\mathrm{d}\bar{s}^2 = \{\delta_{ik} + \partial_i u_k + \partial_k u_i + (\partial_i u_j)(\partial_k u_j)\} \, \mathrm{d}x_i \mathrm{d}x_k . \tag{2.25}$$

This is the squared distance of the neighboring points after deformation. It was $\mathrm{d}s^2 = \delta_{ik} \mathrm{d}x_i \mathrm{d}x_k$ in the relaxed state.

We therefore describe the deformation of a solid medium by

$$2S_{ik} = \partial_i u_k + \partial_k u_i + (\partial_i u_j)(\partial_k u_j), \tag{2.26}$$

such that

$$\mathrm{d}\bar{s}^2 = \mathrm{d}s^2 + 2S_{ik} \mathrm{d}x_i \mathrm{d}x_k \tag{2.27}$$

holds true. $S_{ik} = S_{ik}(t, \boldsymbol{x})$ is the strain tensor field.

If the displacement is achieved by a rigid rotation and a translation,

$$\bar{\boldsymbol{x}} = \boldsymbol{a} + R\boldsymbol{x} \text{ or } \boldsymbol{u} = \boldsymbol{a} + (R - I)\boldsymbol{x}, \tag{2.28}$$

where $\boldsymbol{a}$ is a constant vector and R a constant orthogonal matrix, we work out

$$2S_{ik} = (R - I)_{ik} + (R - I)_{ki} + (R - I)_{ij}(R - I)_{kj} = 0. \tag{2.29}$$

This result is evident when looking at Eq. (2.27). Indeed, the strain tensor field describes deformation. A rigid translation or rotation of a medium does not produce strain.

Note that the displacement gradient $\partial_i u_k$ is dimensionless. For real solids, these gradients are small, and the quadratic contribution $(\partial_i u_j)(\partial_k u_j)$ to Eq. (2.25) may be neglected. Likewise, the square root of Eq. (2.27) may be approximated by

$$\mathrm{d}\bar{s} = \mathrm{d}s + S_{ik}\mathrm{d}x_i\mathrm{d}x_k \text{ with } S_{ik} = \frac{\partial_i u_k + \partial_k u_i}{2}. \tag{2.30}$$

ds was the distance between two neighbors in the relaxed state of the medium. d$\bar{s}$ is the distance between the same material points after a deformation which sends $\boldsymbol{x}$ to $\boldsymbol{x} + \boldsymbol{u}(t, \boldsymbol{x})$. Relation (2.29) is an approximation, it holds true for small displacement gradients, $|\partial_i u_k| \ll 1$. It should not be used if large deformations of rubber-like substances are to be modeled.

The mapping $\boldsymbol{x} \to \bar{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{u}(t, \boldsymbol{x})$ changes the volume element dV into

$$\mathrm{d}\bar{V} = \mathrm{d}V \, \frac{\partial(\bar{x}_1, \bar{x}_2, \bar{x}_3)}{\partial(x_1, x_2, x_3)}, \tag{2.31}$$

where the quotient denotes the functional determinant. If terms which are quadratic or of higher order in $\partial_i v_k$ are neglected, we obtain the following expression

$$\frac{\mathrm{d}\bar{V}}{\mathrm{d}V} = 1 + \partial_j u_j. \tag{2.32}$$

This can be written as

$$\frac{\mathrm{d}\bar{V} - \mathrm{d}V}{\mathrm{d}V} = S_{jj}. \tag{2.33}$$

The relative volume change due to deformation is equal to the trace of the strain field.

2.2.2 Hooke's Law

Without stress there is no strain. Hooke's law says that little stress will produce little strain. Put otherwise, strain is proportional to stress.

The most general linear relation reads

$$S_{ij} = \Lambda_{ijkl} T'_{kl}. \tag{2.34}$$

This would mean 84 elasticity constants. However, the strain tensor as well as the stress tensor are symmetric. Moreover, Λ_{ijkl} can be defined as a second derivative of a free energy with respect to T_{ij} and T_{kl} which assures $\Lambda_{ijkl} = \Lambda_{klij}$. This reduces the number of elasticity constants to maximally 21.

This is a horribly large number, and it pertains to mono-crystals of the most complex symmetry only. In practice, matter in its solid state, like steel, concrete, ice and the like are mixtures of micro-crystallites which are oriented randomly and let the material appear isotropic. In the following we concentrate on isotropic solids, but we bear in mind that materials like wood or mono-crystalline $\mathrm{LiNbO_3}$ are not isotropic.

A linear relation between strain and stress for an isotropic material is described by two constants. The stress tensor itself as well as the unit tensor multiplied be the trace of the stress tensor are independent symmetric second rank tensor. Following tradition, we write

$$S_{ik} = \frac{1+\nu}{E} T'_{ik} - \frac{\nu}{E} \delta_{ik} T'_{jj}. \tag{2.35}$$

Note that ν is a dimensionless number. The constant E has the dimension of pressure, or energy density, just as T_{jk}. It is called the elasticity constant, or Young's modulus, and ν is known as Poisson's ratio.

We will work out examples which demonstrate that the elasticity constant E must be positive. We will likewise demonstrate that Poisson's ratio is restricted to values between 0 (very stiff) and 0.5 (rubber, or fluid like):

$$0 \le \nu \le \frac{1}{2}. \tag{2.36}$$

This simply says that an elastic medium, if pressed upon, might either not wield or will shrink in volume, but not expand.

Hooke's law for an isotropic elastic medium can also be formulated such that stress appears as a consequence of strain. One has to work out the trace of Eq. (2.34),

$$S_{jj} = \frac{1-2\nu}{E} T'_{jj}, \tag{2.37}$$

and obtains

$$T'_{ik} = \frac{E}{(1+\nu)} \left\{ S_{ik} + \frac{\nu}{1-2\nu} \delta_{ik} S_{jj} \right\}. \tag{2.38}$$

Stress is linearly related with strain by the compliance tensor which can be read off from Eq. (2.38).

2.2.3 Structural Mechanics

The subject of this huge field is the investigation of structures made of solid elastic material. The purpose of such structures like bridges, houses, cars or spanners is that they remain intact when used. Bridges should not collapse under normal load, houses must be built so that its walls stand up the forces of heavy wind on the roof, a car should be as light as possible but protect its passengers from the effects of collisions in the best possible way, and a spanner should not yield unless excessive torque is applied.

In structural mechanics, static solutions are to be worked out. The momentum balance equation is to be solved for vanishing flow velocity, $\boldsymbol{v} = 0$. Without flow there will be no friction, i.e., T''_{ik} vanishes. At a first glance, a simple thing:

$$\partial_i T'_{ik} + f_k = 0. \tag{2.39}$$

The external forces f_k per unit volume must be compensated by the gradient of the elastic stress tensor.

However, not every solution of Eq. (2.39) is admissible. The reversible contribution to the stress tensor T'_{ik} must be derived from a strain tensor by Hooke's law (2.38). And: the strain tensor cannot be anything, but must be derived from a displacement field u_i by Eq. (2.30). We refrain here from rewriting the three equations (2.39) into a system of three coupled partial differential equations for the three displacement fields u_1, u_2, u_3.

A problem is solved if three functions u_k are found which give rise to a strain tensor $S_{ik} = (\partial_i u_k + \partial_k u_i)/2$ and, by Hooke's law, to a stress tensor T'_{ik} which compensates external forces according to Eq. (2.39). And: the solution must match the boundary conditions of the problem at hand.

The next thing should be to investigate the stress tensor field $T'_{ik} = T'_{ik}(\boldsymbol{x})$. Note that in structural mechanics only *static* solutions are studied, therefore the time argument is absent.

The stress tensor is real and symmetric and can therefore be diagonalized by an orthogonal coordinate transformation, at least locally. T'_{ik} has three eigenvalues $T^1 = T^1(\boldsymbol{x})$, $T^2 = T^2(\boldsymbol{x})$, and $T^3 = T^3(\boldsymbol{x})$. Negative values denote pressure, positive values indicate stress.

Now, for each material there is an upper limit of pressure or stress which it can support. If these limits are exceeded, the material will yield irreversibly, it will break. Concrete, for example, can support a large pressure, but is feeble with respect to stress. Therefore, steel rods are embedded to strengthen its ability to withstand stress.

The main goal of a structural mechanical analysis is to make sure that the structure is safe. This means that nowhere the material's limits of admissible stress or pressure are exceeded. $T^j = T^j(\boldsymbol{x})$ must always be within the limits of allowed values.

We stop here and do not go into details of the stress-strain relation. As a rule of thumb, the linear relation (Hooke's law) is valid up to a certain point (a thousandth of the elasticity module, or so) where unwanted effects set in, such as permanent deformations.

2.2.4 Elastodynamics

In the preceding section we have discussed an elastic medium at rest. We now allow for oscillating material points. The velocity field $v_i = \dot{u}_i$ is the time derivative of the displacement field. Because we resort too Hooke's law, a linear approximation with respect to $\boldsymbol{u}$ and therefore $\boldsymbol{v}$, we may safely neglect the $\partial_i v_i v_k$ term. We therefore obtain the following three partial differential equations:

$$\varrho \ddot{u}_k = \frac{E}{2(1+\nu)} \left\{ \Delta u_k + \frac{1}{1-2\nu} \partial_k \partial_i u_i \right\} . \tag{2.40}$$

This equation which describes the properties of sound in solids does not contain a possible external force. The effect of gravity, for example, is usually negligible. It also refers to an isotropic medium. Moreover, friction has not yet been incorporated. We shall demonstrate in Chap. 4 that there are transversal and longitudinal solution with different propagation constants as well as surface acoustic waves (SAW). Note that E and ν in Eq. (2.40) are adiabatic values which will differ from the values in Eq. (2.38). The former refer to constant entropy (no heat exchange), the latter to constant temperature.

2.2.5 Summary

A solid, or elastic medium can support shear stress even if at rest. If deformed moderately, it will return to its normal state when relaxed. Hooke's law describes the linear relationship between stress and strain. The latter is a tensor field describing the deformation of an elastic medium. We discuss the discipline of structural mechanics, a discipline of physics or engineering science dedicated to the stability of structures made of elastic solid media. From spanners to skyscrapers. We also talk about elastic waves.

2.3 Heat Conduction

Although used widely, the title of this section is not quite correct. It suggests that a physical quantity called heat is transported via conduction. In fact, it is internal energy which is conducted. Recall that energy, in the context of continuum physics, is made up of kinetic energy, potential energy, and a rest which is called internal energy. The first refers to the motion of material points as a whole, the second to its energy in an external gravitational or electric potential. The last contribution to energy takes into account the motion of particles within a resting material point. Also recall that a material point is small on an engineer's point of view but still contains a huge number of particles. There are so many particles that the laws of thermodynamics for infinitely many are applicable.

2.3.1 Fourier's Law

The balance equation for internal energy U reads

$$\varrho \, \mathrm{D}_t \, u = -\partial_i \, J^{\mathrm{u}}_i + T_{ik} G_{ik} + J^{\mathrm{e}}_i E_i \,. \tag{2.41}$$

Here ϱ is the mass density of the medium and u denotes the specific[9] internal energy. D_t stands for the substantial time derivative, a change in time as observed by a co-moving observer. The conduction contribution to the internal energy current density is denoted as $\boldsymbol{J}^{\mathrm{u}}$. We call it the heat current density. How it depends on other fields is the subject of this section.

There are at least two mechanisms for the production of internal energy. One is friction, as described by $T_{ik} G_{ik}$. If there is stress (T_{ik}) and a velocity gradient (G_{ik}), then internal energy will be produced. We have discussed this in the section on *fluid media*. Another one is $J^{\mathrm{e}}_i E_i$. If an electric current flows in the presence of an electric field, then internal energy will be produced as well. We shall discuss this effect later in the section on *charge transport*. There are more sources of internal energy production, for instance by radioactivity. Here we concentrate on a relation between the heat current density $\boldsymbol{J}^{\mathrm{u}}$ and other fields which will drive it. Let us assume a situation without electric fields and without concentration gradients first.

Thermodynamic equilibrium is characterized by constant pressure, constant temperature, constant electric potential and constant chemical potentials. Assume that one condition is not met, namely constant temperature. As a consequence, internal energy will flow from warmer into colder regions. A vanishing temperature gradient will cause no flow of internal energy. We postulate that a small temperature gradient will drive a small heat current. So we write, in linear approximation,

$$J^{\mathrm{u}}_i = -\lambda_{ij} \, \partial_j \, T \,. \tag{2.42}$$

This is Fourier's law: the heat current density is a linear function of the local temperature gradient. The coefficients λ_{ij} are constants for small enough temperature differences. If the medium is isotropic, then

$$\lambda_{ij} = \lambda \, \delta_{ij} \tag{2.43}$$

will hold, with a single heat conduction constant λ. Equation (2.42) then reads

$$\boldsymbol{J}^{\mathrm{u}} = -\lambda \, \nabla T \,. \tag{2.44}$$

The heat current density is proportional to the temperature gradient. A positive value of λ guarantees that internal energy flows from warm to colder regions.

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[9] Per unit mass.

This is in accordance with the second law of thermodynamics. Recall expression (1.125) for the volumetric entropy production rate by heat conduction:

$$\pi^{\mathrm{hc}} = J_i^{\mathrm{u}}\,\partial_i \frac{1}{T}. \tag{2.45}$$

We insert Fourier's law (2.41) and find

$$\pi^{\mathrm{hc}} = \frac{1}{T^2}\lambda_{ij}(\partial_i T)(\partial_j T). \tag{2.46}$$

Indeed, the matrix λ_{ij} must be non-negative in order to warrant $\pi^{\mathrm{hc}} \geq 0$. For an isotropic medium this boils down to $\lambda \geq 0$.

2.3.2 More on Heat Conduction

We assume an isotropic medium in order to simplify the discussion. The heat conductivity coefficient λ must not be negative. However, it is not a constant. It depends on composition (i.e., the material under study) and on the local equilibrium parameters such a temperature, pressure, and so forth. The transport of internal energy is a slow process, in general. We need not bother about retardation or non-local effects. Therefore, within a homogeneous material, $\lambda(\boldsymbol{x}) = \lambda(T(\boldsymbol{x}))$ is a good approximation in most situations.

Copper is a good heat conductor. Its heat conduction coefficient at $T = 300$ K is $\lambda = 401\ \mathrm{W\,m^{-1}\,K^{-1}}$. The corresponding values for ice, water and air under normal conditions are 2.18, 0.58 and 0.024, respectively. See the tables of Kaye and Laby [5].

The high thermal conductivity of metals is due to electrons in the conduction band. Isolators, such as ice, transport internal energy via phonon diffusion. In gases, energy transport from one place to another is mediated by collisions of molecules. Liquids are in-between: nearby molecules are correlated just as in crystals, but they behave as dense gases otherwise. Therefore, the metal, crystal, liquid and gas sequence of typical heat transport coefficients is rather plausible.

2.3.3 Heat Equation

Assume a medium at rest, for instance, a solid. Everything shall be in equilibrium except temperature. $T = T(t, \boldsymbol{x})$ depends on the location $\boldsymbol{x}$ and will change with time t.

The specific energy u, in this situation, will depend on space and time because it depends on temperature which depends on space and time. Therefore,

$$\varrho\,\mathrm{D}_t\,u = \varrho\dot{u} = \varrho\frac{\partial u}{\partial T}\,\dot{T} \tag{2.47}$$

holds true.

The partial derivative of the specific[10] internal energy with respect to temperature is the specific heat of the material under discussion. It is usually abbreviated by c. With Fourier's law we arrive at

$$\varrho c\,\dot{T} = \partial_i\,\lambda\,\partial_i\,T + \pi^{\mathrm{u}}. \tag{2.48}$$

Here ϱ is the mass density, c the specific heat, T the temperature, and λ the heat conductivity coefficient. π^{u} denotes the amount of internal energy produced per unit time and per unit volume. All these quantities are fields depending on time and location. Equation (2.48) is the so-called heat equation.

If there is no internal energy production and if mass density ϱ, specific heat c and the heat conduction coefficient λ may be considered constant, the heat equation simplifies to

$$\dot{T} = \kappa\varDelta T, \tag{2.49}$$

with

$$\kappa = \lambda / c\varrho. \tag{2.50}$$

$\varDelta = \partial_i\,\partial_i$ stands for the Laplacian differential operator. Equation (2.49) is applicable only if the temperature differences, for a given problem, are small. κ is called *thermal diffusivity* by many authors.

2.3.4 Summary

Heat conduction is short for the conduction of internal energy. It is caused by a temperature gradient if all other equilibrium parameters are constant. We explain Fourier's law and comment on some subtle points, in particular, why metals, other solids, liquids and gases exhibit wildly different heat conduction coefficients. We also digress on the validity of the so called heat equation.

2.4 Diffusion

We discuss in this section the phenomenon that particles of a given kind flow with another velocity than the center of mass. We recapitulate the appropriate balance equation and let us guide by the entropy production expression to formulate a material equation. This then is rewritten into the well-known diffusion equation.

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[10] Recall that specific refers to unit mass.

2.4.1 Diffusion Currents

We have denoted by $n^a = n^a(t, \boldsymbol{x})$ the density of particles of kind a. Note that we cannot enumerate the particles itself because they are indistinguishable. Particles of species a flow with a velocity $\boldsymbol{v}^a = \boldsymbol{v}^a(t, \boldsymbol{x})$. The diffusion currents are

$$\boldsymbol{J}^a = n^a\,(\boldsymbol{v}^a - \boldsymbol{v}). \tag{2.51}$$

It is the conduction contribution $\boldsymbol{J}(N^a)$ associated with the number N^a of particles of kind a. The balance equation for N^a may be written in different forms, one is

$$\partial_t n^a + \partial_i n^a v + \partial_i J_i^a = \pi^a, \tag{2.52}$$

where the volumetric production rates is given by

$$\pi^a = \sum_r \Gamma^r \nu^{ra}. \tag{2.53}$$

It describes the appearance or disappearance of particles due to chemical reaction which are labeled by an index r. Γ^r is the number of such reactions per unit time and unit volume. In one reaction ν^{ra} particles of kind a are produced or vanish, respectively. See Table 1.1 for an example.

2.4.2 Chemical Potential

If two systems have the same temperature T, they do not exchange energy. Consider likewise two systems the volume of the first may grow or shrink at the expense of the second. If two such systems have the same pressure p, they do not exchange volume. And if the two systems have the same temperature and pressure, but may exchange particles of kind a, they will not do so if their chemical potentials μ^a are equal. T, p and the μ^a are equilibrium parameters.

Just look at the expression

$$\pi^{\text{df}} = -\sum_a J_i^a\,\partial_i \frac{\mu^a}{T} \tag{2.54}$$

for the volumetric entropy production rate related with diffusion. Like all other contributions it is a sum of products. The first factor is a flux, the second would vanish in an overall equilibrium situation.

We therefore write provisionally

$$\boldsymbol{J}^a = -\sum_b \Lambda^{ab}\,\nabla \frac{\mu^b}{T}. \tag{2.55}$$

A non-negative matrix of coefficients Λ^{ab} guarantees that the second law of thermodynamics is respected. By the way, the matrix Λ must also be symmetric because of Onsager's relations. We come back to this issue in the following chapter.

2.4.3 Diffusion Equation

We now specialize to a much simpler situation where only on species of particles is not in overall equilibrium. We refer to it by n, $\boldsymbol{J}$ and μ: to its density, its diffusion current and its chemical potential. Moreover, the temperature equilibrium is usually attained much faster than the equilibrium with respect to diffusion. Therefore we assume a constant temperature. Equation (2.55) then simplifies to

$$\boldsymbol{J} = -\frac{\Lambda}{T}\,\nabla\,\mu. \tag{2.56}$$

Λ is a positive coefficient.

The chemical potential has a gradient because the particle density is not yet constant, so we write

$$\boldsymbol{J} = -D\nabla n, \tag{2.57}$$

where the diffusion constant D is defined as

$$D = \frac{\Lambda}{T}\,\frac{\partial\mu}{\partial n}. \tag{2.58}$$

If there are no chemical reactions, and if the medium in which the diffusing particles are suspended is at rest, we have to solve

$$\partial_t n = \partial_i\, D\, \partial_i n, \tag{2.59}$$

the diffusion equation. If the particle density gradients are small, this simplifies even more to

$$\dot{n} = D\,\Delta n. \tag{2.60}$$

Note the similarity with the heat equation. After all, heat propagation in dense media is nothing else than phonon diffusion. Equation (2.59) is occasionally called *Fick's law*.

2.4.4 Digression on Open Systems

We know that Λ in Eq. (2.58) is positive, and the temperature T as well. In order to show that also the diffusion constant D is positive, we must provide an argument why the particle density n increases with μ, the chemical potential.

Denote by $H = H(\lambda)$ the Hamiltonian[11] of the system and by N the particle number operator. The free energy of such an open[12] system is

$$F(T,\lambda,\mu) = -k_{\mathrm{B}}T \,\ln\, \mathrm{tr}\, \mathrm{e}^{\,(\mu N - H)/k_{\mathrm{B}}T}\,. \tag{2.61}$$

Temperature T and chemical potential μ are Lagrange multipliers.

When looking for the maximum of the entropy functional,

$$S(G) = \max_{W} S(W) \text{ where } S(W) = -k_{\mathrm{B}}\,\mathrm{tr}\, W \ln W, \tag{2.62}$$

the mixed state W is confined by $\mathrm{tr}\, W = 1$, $\mathrm{tr}\, WH = U$ and $\mathrm{tr}\, WN = \bar{N}$. The corresponding three Lagrange multipliers are the free energy F, the temperature T, and the chemical potential μ.

One easily calculates

$$\frac{\partial F}{\partial \mu} = -\langle\, N \,\rangle \tag{2.63}$$

and

$$\frac{\partial^2 F}{\partial \mu^2} = -\frac{\langle\, N^2 \,\rangle - \langle\, N \,\rangle^2}{k_{\mathrm{B}}T}. \tag{2.64}$$

If we refer to unit volume, the above two results show that indeed

$$\frac{\partial n}{\partial \mu} \ge 0 \tag{2.65}$$

holds true because of $\langle\, N^2 \,\rangle \ge \langle\, N \,\rangle^2$.

2.4.5 Summary

Diffusion currents of particles are driven by gradients of their chemical potentials weighted with the inverse temperature. However, heat conduction is usually much faster than diffusion. So we specialized on diffusion at constant temperature. We derived the diffusion equation and brought forward an argument why the diffusion constant D must be positive. These findings are supported by a more detailed study of *Brownian motion* in Chap. 4. When combined with chemical reactions, diffusion may lead to astonishing solutions, as discussed in the article on *Reactions and Diffusion*.

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[11] λ stands for the external parameters.

[12] The number of particles within the system is not fixed.

2.5 Charge Transport

In this section we will discuss the various contributions to the electric charge density and the electric charge current density. Ohm's law is formulated for the electrochemical potential.

2.5.1 The Electromagnetic Field in Matter

Let us recall Maxwell's equations for the electromagnetic field $\boldsymbol{E}, \boldsymbol{B}$:

$$\epsilon_0 \nabla \cdot \boldsymbol{E} = \varrho^{\mathrm{e}} \,, \tag{2.66}$$

$$\nabla \cdot \boldsymbol{B} = 0 \,, \tag{2.67}$$

$$\frac{1}{\mu_0} \nabla \times \boldsymbol{B} = \epsilon_0 \dot{\boldsymbol{E}} + \boldsymbol{j}^{\mathrm{e}} \,, \tag{2.68}$$

$$\nabla \times \boldsymbol{E} = -\dot{\boldsymbol{B}} \,. \tag{2.69}$$

Assume that a continuum is exposed to an electromagnetic field. One effect will be that matter gets polarized: there is a certain density of electric dipole moment which we denote by $\boldsymbol{P}$. The negative divergence of this polarization is a contribution to the charge density,

$$-\nabla \cdot \boldsymbol{P} = \varrho^{\mathrm{p}}. \tag{2.70}$$

We call it the polarization charge density. Likewise, there is a current if the polarization changes with time,

$$\dot{\boldsymbol{P}} = \boldsymbol{j}^{\mathrm{p}}. \tag{2.71}$$

Another effect of the electromagnetic field will be magnetization. Denote by $\boldsymbol{M}$ the density of magnetic moments. Its curl is another contribution to the current density,

$$\nabla \times \boldsymbol{M} = \boldsymbol{j}^{\mathrm{m}}. \tag{2.72}$$

In general, the total charge density is made up of two terms,

$$\varrho^{\mathrm{e}} = -\nabla \cdot \boldsymbol{P} + \varrho^{\mathrm{f}}, \tag{2.73}$$

the current density of three,

$$\boldsymbol{j}^{\mathrm{e}} = \dot{\boldsymbol{P}} + \nabla \times \boldsymbol{M} + \boldsymbol{j}^{\mathrm{f}}. \tag{2.74}$$

The superscript “f” stands for “free” or “to be freely manipulated”, in contrast to “p” (enforced by polarization) or “m” (enforced by magnetization).

This is a vicious circle: it is the electric field which causes polarization, the latter then contributes to the electric charge density which in turn must be known for working out the electric field. The same applies to the magnetic induction field.

The well known way out is to define auxiliary fields, the dielectric displacement

$$\boldsymbol{D} = \epsilon_0 \boldsymbol{E} + \boldsymbol{P} \tag{2.75}$$

and the magnetic field strength

$$\boldsymbol{H} = \frac{1}{\mu_0}\boldsymbol{B} - \boldsymbol{M}. \tag{2.76}$$

With it Eq. (2.66) may be reformulated as

$$\nabla \cdot \boldsymbol{D} = \varrho^{\mathrm{f}}, \tag{2.77}$$

while Eq. (2.68) changes into

$$\nabla \times \boldsymbol{H} = \boldsymbol{j}^{\mathrm{f}} + \dot{\boldsymbol{D}}. \tag{2.78}$$

Equations (2.67) and (2.69) remain unchanged.

Now only the density and the current density of free charges show up. The prize to be paid is that we have to cope with two more vector fields. We require additional functional relations between the displacement and the electric fields on the one hand and the magnetic and induction fields on the other. Such relations are material equations because they depend on the material under investigation.

By the way, differentiating Eq. (2.77) with respect to time and working out the divergence of Eq. (2.78) shows that not only charge is a conserved quantity, but also the free charge,

$$\partial_t \varrho^{\mathrm{f}} + \nabla \cdot \boldsymbol{j}^{\mathrm{f}} = 0. \tag{2.79}$$

We will not discuss magnetization further since magnetism was ignored in the preceding sections. For an isotropic dielectric medium and for quasi-static fields

$$\boldsymbol{D} = \epsilon\epsilon_0 \boldsymbol{E} \tag{2.80}$$

is a good approximation. ϵ is the relative dielectric permittivity which can be as large as 80 (for water at 20°C) and even larger.

In Chap. 3 we go beyond this, then also rapidly varying electric fields are dealt with.

2.5.2 Contributions to the Electric Current Density

We have presented two decompositions of the electric current density, one based on Maxwell's equations, the other within the framework of continuum mechanics:

$$\boldsymbol{j}^{\mathrm{e}} = \dot{\boldsymbol{P}} + \boldsymbol{j}^{\mathrm{f}} = (-\nabla \boldsymbol{P} + \varrho^{\mathrm{f}})\,\boldsymbol{v} + \boldsymbol{J}^{\mathrm{e}\,\prime} + \boldsymbol{J}^{\mathrm{e}\,\prime\prime}. \tag{2.81}$$

The first sum describes the decomposition into bound and free charges. The second sum has four contributions, two for convection and two for conduction. We interpret these expressions as follows.

- $\varrho^{\mathrm{f}}\,\boldsymbol{v}$ is the convection of free charges.
- $\boldsymbol{J}^{\mathrm{e}\,\prime} = \dot{\boldsymbol{P}} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{P} = D_t\boldsymbol{P}$ is the substantial time derivative of the polarization. It describes the reversible (or elastic) charge transport by conduction.
- The remainder $\boldsymbol{j}^{\mathrm{f}} = \boldsymbol{J}^{\mathrm{e}\,\prime\prime}$ is responsible for the irreversible (or inelastic) charge transport by conduction.

The situation simplifies if the medium under discussion is at rest. Then there is no charge transport by convection. Partial and substantial time derivatives coincide, and we may write

$$\boldsymbol{j}^{\mathrm{e}} = \boldsymbol{J}^{\mathrm{e}} = \dot{\boldsymbol{P}} + \boldsymbol{J}^{\mathrm{e}\,\prime\prime}. \tag{2.82}$$

2.5.3 Ohm's Law

Let us talk about the normal case that charge is transported by electrons. There are two different causes for electrons to move.

One is the drag of an electric field strength $\boldsymbol{E}$ which exerts a force $-e\boldsymbol{E}$ on an electron. We here discuss quasi-static electric fields, therefore the electric field strength can be derived from a potential ϕ^{e} by $\boldsymbol{E} = -\nabla\phi^{\mathrm{e}}$.

The second cause is diffusion. If the chemical potential μ^* of free electrons has a gradient, it will make these electrons to move whereby each electron carries the charge $-e$. Therefore, the electrostatic potential must be supplemented by the chemical potential divided by the charge $-e$. We call

$$\psi = \phi^{\mathrm{e}} - \frac{\mu^*}{e} \tag{2.83}$$

the electrochemical potential.

Ohm's law states that the irreversible contribution to the electric conduction current is proportional to the negative gradient of the electrochemical potential:

$$J_i^{\mathrm{e}\,\prime\prime} = -\sigma_{ik}\,\partial_k\psi. \tag{2.84}$$

σ_{ik} is the conductivity tensor. We will prove in Chap. 3 that it is symmetric if i and k are exchanged and if an external quasi-static magnetic field is inverted.

The conductivity tensor σ_{ik} is also positive. This follows from the second law of thermodynamics. We have silently assumed that the medium has constant temperature, therefore the entropy production rate per unit volume is

$$\pi(S) = -\frac{1}{T} J_i^{\mathrm{e}\,\prime\prime} \partial_i \psi = \frac{1}{T} (\partial_i \psi)\, \sigma_{ik}\, (\partial_k \psi). \tag{2.85}$$

If there are no chemical reactions which produce differences in the chemical potential for electrons, and if the medium is isotropic, Ohm's law says

$$\boldsymbol{j}^{\mathrm{e}} = \sigma \boldsymbol{E}. \tag{2.86}$$

Note that there were quite a few assumptions which lead to this simple form of Ohm's law.

In older textbooks you may read of an *electromotive force* which pumps electrons. Such pumps may be batteries, photovoltaic cells and voltage differences.

2.5.4 Summary

Charge transport means that charged particles change their location: electrons, holes or ions. A classification in terms of bound and free charges and their corresponding current densities is one subject. Another one is the classification in terms of the general scheme of continuum physics: convection and conduction, the latter reversible or irreversible. We explain how these different points of view are to be reconciled. Electrons, holes or ions move because they are dragged by an electric field, or because they diffuse. The two effects are described by the electrochemical potential. Ohm's law states that the irreversible conduction of electrons is proportional to the negative gradient of the electrochemical potential. The conductivity tensor is symmetric and positive. The subject will be reconsidered in Chap. 3. Also see the article on *Ohms Law and the Hall effect*.

2.6 Thermoelectric Effects

In this section we will discuss cross effects. There is more that one generalized force and their are many corresponding fluxes. The fluxes depend linearly on the generalized forces, but the matrix of kinetic coefficients is neither diagonal nor arbitrary. We postpone a detailed discussion of the underlying Onsager relations to Chap. 3. In order to be specific we discuss a solid electric conductor such that electric charge and internal energy may be transported.

2.6.1 Simultaneous Heat and Charge Transport

We specialize to a solid electrical conductor with non-vanishing electrical and heat conductivities. The possible fluxes are the electric current density $\boldsymbol{J}^{\mathrm{e}}$ and the heat current density $\boldsymbol{J}^{\mathrm{u}}$.

If there were no charge transport, the temperature gradient ∇T would drive the heat current. And vice versa, if there were no temperature gradient and no heat current, the gradient of the electrochemical potential $\nabla\psi$ would drive the electric current. There will be cross effects if both is allowed, charge and heat conduction.

Mobile electrons, which are referred to by an asterisk superscript, will transport both charge and internal energy. On the other hand, diffusion of phonons[13] causes internal energy transport only. Since each quasi-free electron carries a negative unit charge we may write

$$\boldsymbol{J}^{\mathrm{e}} = -e\boldsymbol{J}^{*}. \tag{2.87}$$

The electrochemical potential is given by

$$\psi = \phi^{\mathrm{e}} - \frac{\mu^{*}}{e}, \tag{2.88}$$

where ϕ^{e} is the ordinary electrostatic potential.

2.6.2 Forces and Fluxes

In global thermodynamic equilibrium the potentials are constant and the current densities vanish. ∇T and $\nabla\psi$ are generalized forces X because they transform as forces with respect to time reversal, $X \to X$. $\boldsymbol{J}^{\mathrm{u}}$ and $\boldsymbol{J}^{\mathrm{e}}$ are generalized fluxes Φ because they transform as $\Phi \to -\Phi$.

One should try to define forces X_a and fluxes Φ_a in such a way that the volumetric entropy production rate reads

$$\pi(S) = \sum_a \Phi_a X_a. \tag{2.89}$$

Since we always discuss only weak deviations from thermodynamic equilibrium, we postulate a linear relationship between fluxes and forces:

$$\Phi_b = \sum_a K_{ba} X_a, \tag{2.90}$$

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[13] Quantized lattice vibrations. Phonons are quasi-particles because they cannot live in free space.

where K_{ba} are kinetic coefficients. This simply expresses the fact that no forces produce zero fluxes and that sufficiently small forces cause small fluxes.

A very specialized form of Onsager's theorem says that the kinetic coefficients form a symmetric matrix. We postpone a discussion of this theorem to Chap. 3. There we derive explicit expressions for the kinetic coefficients and show that the symmetry $K_{ab} = K_{ba}$ is a consequence of time reversal invariance.

2.6.3 Kinetic Coefficients for Heat and Charge Transport

The following contributions to the volumetric entropy production rate do not vanish:

$$\pi(S) = \boldsymbol{J}^{\mathrm{u}} \cdot \nabla \frac{1}{T} - \boldsymbol{J}^{*} \cdot \nabla \frac{\mu^{*}}{T} - \frac{1}{T} \boldsymbol{J}^{\mathrm{e}} \cdot \boldsymbol{E}. \tag{2.91}$$

With the entropy conduction current density

$$\boldsymbol{J}^{\mathrm{s}} = \frac{1}{T} (\boldsymbol{J}^{\mathrm{u}} - \mu^{*} \boldsymbol{J}^{*}) \tag{2.92}$$

one may rewrite the volumetric entropy production rate as

$$\pi(S) = -\frac{1}{T} (\boldsymbol{J}^{\mathrm{s}} \cdot \nabla T + \boldsymbol{J}^{\mathrm{e}} \cdot \nabla \psi). \tag{2.93}$$

This expression has the form Eq. (2.89) up to a common factor which is irrelevant here. We therefore postulate

$$\begin{pmatrix} \boldsymbol{J}^{\mathrm{s}} \\ \boldsymbol{J}^{\mathrm{e}} \end{pmatrix} = - \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} \nabla T \\ \nabla \psi \end{pmatrix}. \tag{2.94}$$

In accordance with Onsager's symmetry relation the off-diagonal elements are equal. Moreover,

$$A \geq 0 \,, \; C \geq 0 \text{ and } AC \geq B^2 \tag{2.95}$$

will guarantee that the second law of thermodynamics is respected.

The electric current density is usually written as

$$\boldsymbol{J}^{\mathrm{e}} = -\sigma (\nabla \psi + \alpha \nabla T). \tag{2.96}$$

We recognize $\sigma = C$, therefore the electric conductivity is always positive. The sign of $\alpha = B/C$ cannot be predicted from first principles. If the temperature is the same everywhere, Eq. (2.96) coincides with Ohm's law (2.84). Moreover, the chemical potential, which depends on temperature and composition, cannot have a gradient in a homogeneous medium. We may then write $\boldsymbol{J}^{\mathrm{e}} = \sigma \boldsymbol{E}$ which is Ohm's law in a narrower sense.

The second relation in Eq. (2.94) can be formulated as

$$\boldsymbol{J}^{\mathrm{u}} = -\lambda \nabla T + \gamma \boldsymbol{J}^{\mathrm{e}}. \tag{2.97}$$

Without electric current we obtain Fourier's law $\boldsymbol{J}^{\mathrm{u}} = -\lambda \nabla T$. The heat conductivity $\lambda = T(A - B^2/C)$ is guaranteed to be positive.

An additional electric current causes additional heat transport. However, the sign of γ cannot be derived from a general rule, just like that of α in Eq. (2.96). The coefficients γ in Eq. (2.97) and α in Eq. (2.96) are related by

$$\gamma = T\alpha - \frac{\mu^*}{e}. \tag{2.98}$$

You will find further details in article on *Thomson, Seebeck and Peltier effect*.

2.6.4 Summary

In general, if there are many driving forces and equally many fluxes, they are related by a matrix K of kinetic coefficients. This matrix is symmetric provided that forces and fluxes are defined in such a way that the volumetric entropy production rate is a sum of flux times force products. As an example of this Onsager relation we study an electric conductor of homogeneous composition. There are two driving forces, namely the electric field strength and the temperature gradient. The corresponding fluxes are the electric and the heat current densities. Besides Ohm's and Fourier's law, there are cross effects.

Chapter 3
Linear Response Theory

So far we have discussed bulk matter as a collection of material points which are always in thermodynamic equilibrium with neighboring material points. The parameters which determine the equilibrium state, such as temperature, pressure or chemical potentials, may vary from location to location and with time. They are, however, well defined for each material point.

There are situations where this assumption is unjustified. Just think of the interaction of light with matter. The electric field strength of a light wave changes so rapidly that micrometer sized material points have no time to follow. They will always be away from thermodynamic equilibrium.

In this chapter we discuss the perturbation of matter by a rapidly varying external parameter and the response to it in first, or linear approximation. We develop the theory in full generality, but specialize later to the field of optics.

3.1 Statistical Thermodynamics

We summarize the basics of quantum theory and explain the concept of mixed states. Entropy is a measure of how much a state is mixed. The state of a well isolated system becomes mixed more and more until its entropy is maximal. This state of maximal entropy, the Gibbs state, describes the system when it is in equilibrium with its environment.

3.1.1 Quantum Theory

A physical system is represented by a Hilbert space $\mathcal{H}$. Its elements—we call them vectors—can be added and multiplied by scalars, here always complex numbers. For $f, g \in \mathcal{H}$ there is a scalar product (g, f) which is linear in the right hand side. This means $(g, \alpha_1 f_1 + \alpha_2 f_2) = \alpha_1(g, f_1) + \alpha_2(g, f_2)$. The scalar product shall

P. Hertel, *Continuum Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-642-29500-3_3,

obey $(g, f) = (f, g)^*$ where the asterisk denotes complex conjugation. Recall that $\|f\|^2 = (f, f)$ is never negative. It vanishes if and only if f is the zero vector.

Observables, states and symmetries are represented by linear operators. Such a linear operator $A : \mathcal{H} \to \mathcal{H}$ maps the Hilbert space $\mathcal{H}$ onto itself such that the linear combination $f = \alpha_1 f_1 + \alpha_2 f_2$ is mapped into $Af = \alpha_1 A f_1 + \alpha_2 A f_2$. Linear operators can be multiplied by a scalar, they can be added, and they can be multiplied according to $(BA)f = B(Af)$.

For each linear operator $A : \mathcal{H} \to \mathcal{H}$ there is an adjoint linear operator $A^\dagger : \mathcal{H} \to \mathcal{H}$ for which

$$(g, Af) = (A^\dagger g, f) \tag{3.1}$$

holds true, for all vectors f and g. Note

$$(BA)^\dagger = A^\dagger B^\dagger. \tag{3.2}$$

An operator which commutes with its adjoint,

$$[A^\dagger, A] = A^\dagger A - A A^\dagger = 0, \tag{3.3}$$

is said to be normal. Normal operators have a remarkable property: they can be diagonalized. There is a complete orthonormal system $f_1, f_2, \dots$ of vectors such that

$$A f_i = a_i f_i \tag{3.4}$$

holds true. The $f_i \in \mathcal{H}$ are eigenvectors, the $a_i \in \mathbb{C}$ denote the corresponding eigenvalues. The eigenvectors are normalized and pairwise orthogonal:

$$(f_j, f_i) = \delta_{ji}. \tag{3.5}$$

But most important, the orthonormal system is complete. Any $f \in \mathcal{H}$ can be written as

$$f = \sum_i c_i f_i \text{ with } c_i = (f_i, f). \tag{3.6}$$

Observables and States

An observable property of the system under consideration is described by a self-adjoint linear operator M. This means $M^\dagger = M$ from which we infer that M is normal. It can be diagonalized according to

$$M f_i = m_i f_i, \tag{3.7}$$

where the eigenvectors $f_1, f_2, \dots$ form a complete orthonormal system, and the eigenvalues $m_1, m_2, \dots$ are real. Real because of

$$m_i = (f_i, M f_i) = (M^\dagger f_i, f_i) = (M f_i, f_i) = (f_i, M f_i)^* = m_i^*. \tag{3.8}$$

The operator M representing an observable, or measurable property, is called an observable. Linear or angular momentum, location, energy and so forth are examples. The eigenvalues m_i of an observable are real numbers.

So called pure[1] states are represented by normalized vectors $f \in \mathcal{H}$. Any such state may be written as a linear combination according to Eq. (3.6). Because of

$$1 = (f, f) = \sum_{j,i} c_j^* c_i (f_j, f_i) = \sum_i |c_i|^2 \tag{3.9}$$

we interpret $|c_i|^2$ as the probability that f_i is contained in f. If M is measured and if the system is in state f_i, the measurement will result in the value m_i. If the system has been prepared in a state f, which is a superposition of the eigenstates f_i, we expect the value

$$\langle M \rangle = \sum_i |c_i|^2 m_i = (f, M f). \tag{3.10}$$

The larger the system, the more it is an oversimplification that a system can be prepared in a pure state as described by a particular vector $f \in \mathcal{H}$. Realistically, a certain observable is measured, and the state is a mixture of the pure eigenstates of that observable. There is a complete orthonormal set of vectors ϕ_i and a corresponding set of probabilities w_i that ϕ_i will be prepared. This information can be expressed by defining a liner operator W such that

$$W \phi_i = w_i \phi_i \tag{3.11}$$

holds true. We call W a mixed state because it describes a mixture of pure states.[2]

The expectation value of the observable M in the mixed state W is

$$\langle M \rangle = \sum_i w_i (\phi_i, M \phi_i) = \sum_i (\phi_i, M W \phi_i) = \operatorname{tr} WM. \tag{3.12}$$

Here $\operatorname{tr} A$ denotes the trace of a linear operator. It is the sum over its diagonal matrix elements $(\chi_i, A\chi_i)$ with respect to a complete orthonormal system $\chi_1, \chi_2, \ldots$ For working out the trace one has to refer to a particular complete orthonormal system, but any other one will lead to the same value. Note that

$$\operatorname{tr} AB = \sum_i (\chi_i, AB\chi_i) = \sum_{ij} (\chi_i, A\chi_j)(\chi_j, B\chi_i) = \operatorname{tr} BA \tag{3.13}$$

holds true. We have made use of it when writing Eq. (3.12).

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[1] We shall soon see why they are called so.

[2] The symbol P in this book is used heavily, for momentum, polarization, and so forth. We therefore denote the probability operator by W, an allusion to the German word *Wahrscheinlichkeit* for probability.

The eigenvalues of a mixed state are probabilities, real numbers. It is therefore self-adjoint, $W = W^\dagger$. Moreover, these eigenvalues sum up to 1 which may be expressed as

$$\operatorname{tr} W = 1. \tag{3.14}$$

In addition, since probabilities can never be negative, a mixed state is represented by a positive linear operator:

$$W \geq 0 \tag{3.15}$$

meaning $(f, Wf) \geq 0$ for all $f \in \mathcal{H}$.

Any linear operator W respecting Eqs. (3.14) and (3.15) represents a state.

Let us mention in passing a simple consequence of Eq. (3.12). Denote by H the energy observable. In a coordinate frame where the center of mass of the system is a rest the energy expectation value is called *internal energy* and traditionally designated as $U = \operatorname{tr} WH$. We deduce from Eq. (3.12) the following relation

$$\mathrm{d}U = \operatorname{tr} \mathrm{d}WH + \operatorname{tr} W\mathrm{d}H = \mathrm{d}Q + \mathrm{d}A. \tag{3.16}$$

The internal energy may change because of two causes. Either the state or the energy observable changes. The first contribution is called heat, the second work.[3] This simple consequence of Eq. (3.12) is known as the *First law of thermodynamics*.

3.1.2 Entropy

We now set out to define a measure for how much a state is mixed.

We prepare the system according to the prescription (3.11): the pure state ϕ_i occurs with probability w_i. It has been proven over and over again: single measurements are not predictable. Nature seems to throw dices. Only a long series of measurements, an experiment, provides reliable results.

Assume we have performed an experiment by measuring the state N times. The protocol of the experiment could be $\phi_2, \phi_5, \phi_2, \phi_2, \phi_1, \dots$ The state ϕ_i was encountered n_i times, where $\sum_i n_i = N$.

There are

$$\Omega = \frac{N!}{n_1! \cdot n_2! \cdot \dots} \tag{3.17}$$

different protocols which are compatible with

$$w_i \approx \frac{n_i}{N}. \tag{3.18}$$

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[3] Since the symbol W had to be assigned to the probability operator, we here denote work by dA alluding to *Arbeit*, German for work.

Before performing the experiment we just know the probabilities w_i for the occurrence of the state ϕ_i. *Afterwards* we know more, namely the protocol. The information gain, measured in bits, is $\log_2 \Omega$. This is the number of yes/no questions which one must ask in order to learn which protocol has been realized out of Ω possible protocols. With Stirling's formula $\log n! \approx n \, \log n$ we find

$$\frac{\log_2 \Omega}{N} \to -\sum_i w_i \log_2 w_i = -\operatorname{tr} W \log_2 W, \tag{3.19}$$

with $N \to \infty$. For sufficiently many measurements, the information gain of an experiment is proportional to the number of measurements. It depends on the probabilities w_i only.

If all probabilities vanish up to one, which is 1, we have a mixture with just one contribution. This characterizes a non-mixed, or pure state. Repeating the measurement will always yield the same result, and no information can be gained. As it should be, the right hand side of Eq. (3.19) vanishes.

Since $x \to -x \log x$ on $x \in [0, 1]$ is a non-negative concave function, the right hand side of Eq. (3.19) will never be negative. It vanishes for pure states and is positive otherwise. For historical reasons we replace the *logarithmus dualis* by the natural logarithm and multiply with Boltzmann's constant. The result is the entropy of the state W:

$$S(W) = -k_\mathrm{B} \operatorname{tr} W \, \ln W. \tag{3.20}$$

It serves as the measure of how much a mixed state is mixed.

Note that two mixed states W_1 and W_2 can be further mixed by

$$W = (1-\alpha)W_1 + \alpha W_2 \text{ with } 0 \le \alpha \le 1. \tag{3.21}$$

Obviously this is a state because $W \ge 0$ and $\operatorname{tr} W = 1$ are fulfilled if the same is true for W_1 and W_2. It can be shown that the following inequality holds true:

$$S(W) \ge (1-\alpha)S(W_1) + \alpha S(W_2), \tag{3.22}$$

with W of Eq. (3.21). The entropy of the mixed state is larger than or equal to the mixture of entropies. Mixing increases entropy.

By the way, the entropy of a state W depends on its eigenvalues w_i only, the complete orthonormal system $\phi_1, \phi_2, \ldots$ is irrelevant. This complies with the axiom that all states are *a priori* equally probable.

3.1.3 Equilibrium

For an ideally isolated system the state W_t obeys the Schrödinger equation

$$\frac{\mathrm{d}W_t}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\,[W_t, H], \tag{3.23}$$

where H is the energy observable, or energy. The solution

$$W_t = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}tH} W_0 \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}tH} \tag{3.24}$$

is a unitary transformation which preserves the eigenvalues of W_t. We conclude that the Schrödinger equation (3.22) preserves entropy. For an autonomous[4] system the entropy of states is conserved.

A sufficiently large system, however, cannot be isolated for a long time from its environment. One may well hinder it from exchanging energy with its environment, but the influence of the surrounding world on the time development of the system cannot be neglected. The second law of thermodynamics, loosely speaking, states that the degree of mixing, or disorder, increases more and more, although there is no exchange of energy. We speak of a well, but not ideally isolated system.

The entropy of a well isolated system increases in the course of time until its maximal value has been reached. The corresponding state G describes the equilibrium between a system and its environment. This Gibbs state G is characterized by

$$S(W) \le S(G) \text{ with } \operatorname{tr} WH = U. \tag{3.25}$$

G must be such that

$$\mathrm{d}S = -k_{\mathrm{B}} \operatorname{tr} \mathrm{d}W \ln G \tag{3.26}$$

vanishes together with $\mathrm{d}U = \operatorname{tr} \mathrm{d}WH$ and $\operatorname{tr} \mathrm{d}W$. By multiplying with appropriate Lagrange multipliers F and T we arrive at

$$G = \mathrm{e}^{(F-H)/k_{\mathrm{B}}T}. \tag{3.27}$$

The Lagrange parameter F, the free energy, is determined by demanding $\operatorname{tr} G = 1$. We find

$$F = -k_{\mathrm{B}}T \ln \mathrm{e}^{-H/k_{\mathrm{B}}T}. \tag{3.28}$$

The second Lagrange parameter, the temperature T, is indirectly determined by solving

$$U = \frac{\operatorname{tr} H \, \mathrm{e}^{-H/k_{\mathrm{B}}T}}{\operatorname{tr} \mathrm{e}^{-H/k_{\mathrm{B}}T}}. \tag{3.29}$$

The right hand side of Eq. (3.29) increases monotonically with T, and therefore the temperature is uniquely determined.

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[4] Governed by its own laws.

3.1.4 Summary

The pure states and the observable properties of a system are represented by vectors f of a Hilbert space $\mathcal{H}$ and by self-adjoint linear operators $M : \mathcal{H} \to \mathcal{H}$. The larger the system, the more difficult it is to prepare pure states. In fact, for large systems states are always mixtures, or mixed states W. The expectation value $\langle M \rangle = \operatorname{tr} WM$ is a bilinear functional of the observable and the mixed state, and the first law of thermodynamics is a trivial consequence thereof. We argue why the entropy $S = S(W)$ is a good measure of how much a state is mixed. A well, but not ideally isolated system tends to get more and more mixed. The equilibrium between the system and its environment is characterized by maximal entropy, and we explicitly work out the corresponding Gibbs state G. Free energy F and temperature T show up in a natural way.

3.2 Perturbations

The Hamiltonian of the system under discussion may depend on external parameters, $H = H(\lambda)$. Such parameters describe the action of the environment onto the system. However, the feedback, the influence of the system onto its environment, can safely be neglected. If external parameters, such as an electric field, change very slowly, the equilibrium will follow, and we speak of a reversible process. Here we discuss rapid changes. There is not enough time for the system to attain its equilibrium. In this section we will investigate how a system reacts on rapidly varying external parameters, in particular the electric field strength of a light wave.

3.2.1 Interaction Picture

Let us reflect on the role of time within the framework of quantum physics. Up to now we spoke of preparing a system in a state W and then measuring M, the expectation value being $\langle M \rangle = \operatorname{tr} WM$. Time comes into the game by waiting for a time span t between preparing the state and measuring an observable.

Heisenberg has described this situation by regarding "waiting for a time span t and then measuring M" as a new observable, namely M_t.

Since M and M_t have the same eigenvalues, they are related by a unitary transformation,

$$M_t = U_t^\dagger M U_t, \tag{3.30}$$

where U_t obeys

$$U_t^\dagger U_t = U_t U_t^\dagger = I. \tag{3.31}$$

I denotes the unit operator. We call U_t the waiting operator.

Now, first waiting t_1 and then t_2 is the same as waiting a time span $t_1 + t_2$. Consequently,

$$U_{t_2+t_1} = U_{t_2}\, U_{t_1} \tag{3.32}$$

must hold, with $U_0 = I$. These equations are solved by the exponential function:

$$U_t = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} tH} \tag{3.33}$$

with a self-adjoint operator H. We have split off the imaginary unit i such that U_t is unitary with a self-adjoint H. The factor $1/\hbar$ is there for historical reasons: energy $H = \hbar\varOmega$ and angular frequency $\varOmega$ were considered to be different quantities in classical physics.

Note that we may now rewrite Eq. (3.30) as

$$M_t = U_{-t} M U_t \tag{3.34}$$

or as

$$\frac{\mathrm{d}}{\mathrm{d}t} M_t = \frac{\mathrm{i}}{\hbar}\, [H, M_t]. \tag{3.35}$$

In the Heisenberg picture, as described by Eq. (3.34), the expectation value of M in a state W with a time delay of t is given by

$$\langle\, M \,\rangle_t = \operatorname{tr} W M_t. \tag{3.36}$$

Schrödinger thought differently. Preparing a state W and then waiting the time span t defines a state W_t. Because of

$$\langle\, M \,\rangle_t = \operatorname{tr} W M_t = \operatorname{tr} W U_{-t} M U_t = \operatorname{tr} U_t W U_{-t} M = \operatorname{tr} W_t M \tag{3.37}$$

we conclude

$$W_t = U_t W U_{-t}. \tag{3.38}$$

With this, the Schrödinger equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t} W_t = -\frac{\mathrm{i}}{\hbar}\, [H, W_t]. \tag{3.39}$$

Either the observables change with time and the states remain constant, so the Heisenberg picture. Or the observables are constant and the states change with time, so the Schrödinger picture. What can be measured, expectation values, is the same in both pictures.

We have expounded these different views on time because there is a third view, known as the interaction picture, which will help us in tackling perturbations.

In many cases the Hamiltonian H_t can be split into a manageable part H and a small rest V_t which is considered as a perturbation, possibly depending on time.

$$H_t = H + V_t. \tag{3.40}$$

Primarily we think as Schrödinger of states W_t. We transform into the Heisenberg picture with H *only*. If there were no perturbation, the transformed states would not change with time. If there is a small perturbation, the transformed states will depend only weakly on time. Let us now formulate this.

Define

$$W_t(t) = U_{-t} W_t U_t, \tag{3.41}$$

where U_t is given by Eq. (3.33). The following equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t} W_t(t) = -\frac{\mathrm{i}}{\hbar} [V_t(t), W_t(t)] \tag{3.42}$$

has to be fulfilled. Indeed, a small perturbation will result in a small rate of change only. We shall resort to this in the following subsection.

3.2.2 Linear Response

We assume that the system has been in a Gibbs state before the perturbation V_t was switched on:

$$V_t \to 0 \text{ and } W_t \to G \text{ for } t \to -\infty. \tag{3.43}$$

With this initial condition (3.42) can be integrated to

$$W_t(t) = G - \int_{-\infty}^{t} \mathrm{d}s \; \frac{\mathrm{i}}{\hbar} [V_s(s), W_s(s)]. \tag{3.44}$$

It is an integral equation for $t \to W_t(t)$ because this operator-valued function appears on the left hand and on the right hand side. It lends itself to a power series expansion.

Without any perturbation, the solution would be $W_t(t) = G$. We calculate the next best approximation by inserting G into the right hand side of Eq. (3.44) and obtain

$$W_t(t) = G - \int_{-\infty}^{t} \mathrm{d}s \; \frac{\mathrm{i}}{\hbar} [V_s(s), G]. \tag{3.45}$$

This is the linear response to the perturbation by V_t. We will make more out of it.

Let us first undo the transformation to the interaction picture,

$$W_t = G - \int_{-\infty}^{t} \mathrm{d}s \; \frac{\mathrm{i}}{\hbar} [V_s(s-t), G]. \tag{3.46}$$

The expectation value of an observable M is given by

$$\operatorname{tr} W_t M = \operatorname{tr} G M - \int_{-\infty}^{t} \mathrm{d}s \ \operatorname{tr} G \frac{\mathrm{i}}{\hbar} [M, V_s(s-t)], \tag{3.47}$$

or

$$\langle M \rangle_t = \langle M \rangle - \int_{-\infty}^{t} \mathrm{d}s \ \langle \frac{\mathrm{i}}{\hbar} [M, V_s(s-t)] \rangle. \tag{3.48}$$

Expectation values $\langle \dots \rangle$ without a suffix always refer to the Gibbs state.

Let us introduce the age $\tau = t - s$ of a perturbation, so that we may rewrite Eq. (3.48) into

$$\langle M \rangle_t = \langle M \rangle - \int_{0}^{\infty} \mathrm{d}\tau \ \langle \frac{\mathrm{i}}{\hbar} [M(\tau), V_{t-\tau}(0)] \rangle. \tag{3.49}$$

Note that we have time-shifted the expectation value by τ according to Eq. (3.41).

We now specialize to a time-dependent perturbation of the form

$$H_t = H - \sum_k \lambda_k(t) \Lambda_k, \tag{3.50}$$

where $\lambda_k = \lambda_k(t)$ are real valued functions while the Λ_k are observables, i.e., self-adjoint operators. The linear response of such a perturbation is described by

$$\langle M \rangle_t = \langle M \rangle + \int_{0}^{\infty} \mathrm{d}\tau \ \sum_k \langle \frac{\mathrm{i}}{\hbar} [M(\tau), \Lambda_k(0)] \rangle \lambda_k(t-\tau). \tag{3.51}$$

3.2.3 Perturbation by Light

Normal matter consists of nuclei and electrons which we enumerate by $a = 1, 2, \dots$ Particle a is located at $\boldsymbol{x}_a$, has momentum $\boldsymbol{P}_a$, mass m_a and electric charge q_a. The Hamiltonian is well described by

$$H = \sum_a \frac{\boldsymbol{P}_a^2}{2m_a} + \frac{1}{4\pi\epsilon_0} \sum_{b>a} \frac{q_b q_a}{|\boldsymbol{x}_b - \boldsymbol{x}_a|}. \tag{3.52}$$

In electric dipole approximation the interaction with an external electric field $\boldsymbol{E}$ is expressed by

$$H_t = H - \int \mathrm{d}^3 x \, \boldsymbol{P}(\boldsymbol{x}) \cdot \boldsymbol{E}(t, \boldsymbol{x}), \tag{3.53}$$

where

$$\boldsymbol{P}(\boldsymbol{x}) = \sum_a q_a \boldsymbol{x}_a \delta^3(\boldsymbol{x} - \boldsymbol{x}_a) \tag{3.54}$$

is the polarization, a field of observables.

Indeed, the perturbation is of the form (3.50), the "sum" being a sum over the vector components and a spatial integration.

In optics, the polarization caused by a light wave is of particular interest. Hence we have to discuss

$$\langle P_j(\boldsymbol{x}) \rangle_t = \int_0^\infty \mathrm{d}\tau \sum_k \int \mathrm{d}^3 y \, \Gamma_{jk}(\tau, \boldsymbol{x}, \boldsymbol{y}) \, E_k(t - \tau, \boldsymbol{y}), \tag{3.55}$$

where

$$\Gamma_{jk}(\tau, \boldsymbol{x}, \boldsymbol{y}) = \langle \frac{\mathrm{i}}{\hbar} [P_j(\tau, \boldsymbol{x}), P_k(0, \boldsymbol{y})] \rangle. \tag{3.56}$$

Note that $P_j(\tau, \boldsymbol{x}) = U_{-\tau} P_j(\boldsymbol{x}) U_\tau$ is the time-shifted polarization operator.

We add one more assumption, namely that the unperturbed Gibbs state is invariant under spatial translations. In this case the influence functions (3.56) depend on $\boldsymbol{\xi} = \boldsymbol{x} - \boldsymbol{y}$ only, and we may simplify Eq. (3.55) to

$$\langle P_j(\boldsymbol{x}) \rangle_t = \int_0^\infty \mathrm{d}\tau \sum_k \int \mathrm{d}^3 \xi \, \Gamma_{jk}(\tau, \boldsymbol{\xi}) \, E_k(t - \tau, \boldsymbol{x} - \boldsymbol{\xi}) \tag{3.57}$$

and Eq. (3.56) to

$$\Gamma_{jk}(\tau, \boldsymbol{\xi}) = \langle \frac{\mathrm{i}}{\hbar} [P_j(\tau, \boldsymbol{\xi}), P_k(0, 0)] \rangle. \tag{3.58}$$

We have dropped a possible static polarization contribution $\langle P_j(\boldsymbol{x}) \rangle$ since we are interested in optics.

3.2.4 Susceptibility Tensor

Let us Fourier transform the polarization[5] $P_j(t, \boldsymbol{x}) = \langle P_j(\boldsymbol{x}) \rangle_t$,

$$P_j(t, \boldsymbol{x}) = \int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \, \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{e}^{\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{x}} \, \tilde{P}_j(\omega, \boldsymbol{q}). \tag{3.59}$$

The electric field is transformed likewise. We find

$$\tilde{P}_j(\omega, \boldsymbol{q}) = \epsilon_0 \sum_k \chi_{jk}(\omega, \boldsymbol{q}) \, \tilde{E}_k(\omega, \boldsymbol{q}). \tag{3.60}$$

The dielectric susceptibility tensor is

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[5] It should be clear from the context whether we speak of the observable or its expectation value in the perturbed state W_t.

$$\chi_{jk}(\omega, \boldsymbol{q}) = \frac{1}{\epsilon_0} \int_0^\infty \mathrm{d}\tau \int \mathrm{d}^3\xi \; \mathrm{e}^{\mathrm{i}\omega t} \; \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\xi}} \; \Gamma_{jk}(\tau, \boldsymbol{\xi}). \tag{3.61}$$

A perturbation by a plane wave causes a response with the same angular and spatial frequency. The proportionality factor, which depends on ω and $\boldsymbol{q}$, can be calculated, in principle. It is the causal[6] Fourier transform of the influence matrix Γ_{jk} which is the expectation value of a certain commutator in the unperturbed state. This commutator is made up of space- and time-translated polarization observables.

In the remaining sections of this chapter we discuss general properties of the dielectric susceptibility. It consists of a refractive and a dissipative part which are related by a *Dispersion relation*. In the following section on *Fluctuations and dissipation* we show that the dissipative part is never negative and thus causes absorption of field energy by matter. We come very close to a proof of the Second law of thermodynamics. We finally discuss Onsager's relations which are a consequence of time reversal invariance.

3.2.5 Summary

Time in the context of quantum theory is the span between preparing a state and measuring a property. In the Heisenberg picture the observables depend on the time span between preparing and measuring while the Schrödinger picture assumes time-dependent states. The interaction picture is in-between. If the Hamiltonian $H_t = H + V_t$ can be split into a manageable part H and a time-dependent small perturbation V_t, the interaction picture leads to a slowly varying state.

By assuming that the system was in a Gibbs state before V_t was switched on, this initial condition and the equation of motion can be combined to an integral equation which lends itself to a power series expansion in the perturbation. As a special case, the interaction of a light wave with normal matter is studied. One arrives at explicit expressions for the dielectric susceptibility tensor which is the causal Fourier transform of a certain commutator evaluated in the unperturbed Gibbs state.

3.3 Dispersion Relations

A causal function $f = f(\tau)$ vanishes for $\tau \leq 0$. The real and the imaginary part of its Fourier transform are intimately related.

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[6] Only perturbations in the past contribute.

3.3.1 Causal Functions

A real valued causal function f may be written as

$$f(\tau) = \theta(\tau) f(\tau), \tag{3.62}$$

where $\theta = \theta(\tau)$ is the Heaviside step function. It vanishes for $\tau < 0$ and equals 1 for positive arguments. Since it will be used in integrals only, its value for $\tau = 0$ is irrelevant.

The convolution theorem states that the Fourier transform of a product is the convolution of the Fourier transforms. In our case this means

$$g(\omega) = \int \frac{\mathrm{d}u}{2\pi}\, \tilde{\theta}(\omega - u)\, g(u) \tag{3.63}$$

where g denotes the Fourier transform of f.

So, we should work out the Fourier transform of the step function,

$$\tilde{\theta}(\omega) = \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\,\mathrm{i}\omega\tau}. \tag{3.64}$$

This integral makes no sense, so we redefine it as

$$\tilde{\theta}(\omega) = \lim_{0<\epsilon\to 0} \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\,\mathrm{i}(\omega + \mathrm{i}\epsilon)\tau}, \tag{3.65}$$

that is

$$\tilde{\theta}(\omega) = \lim_{0<\epsilon\to 0} \frac{1}{\epsilon - \mathrm{i}\omega}. \tag{3.66}$$

Equation (3.66) says that, when integrating over ω, the pole at $\omega = 0$ should be shipped around in the upper complex half-plane.

Back to Eq. (3.63). Skipping the $\epsilon > 0, \epsilon \to 0$ prefix we may write

$$g(\omega) = \int \frac{\mathrm{d}u}{2\pi\mathrm{i}}\, \frac{g(u)}{u - \omega - \mathrm{i}\epsilon}. \tag{3.67}$$

Let us now add and subtract a term which describes avoiding the pole in the upper half plane:

$$\frac{2}{v - \mathrm{i}\epsilon} = \frac{1}{v - \mathrm{i}\epsilon} + \frac{1}{v + \mathrm{i}\epsilon} + \frac{1}{v - \mathrm{i}\epsilon} - \frac{1}{v + \mathrm{i}\epsilon}. \tag{3.68}$$

Because of

$$\int \frac{\mathrm{d}u}{2\pi\mathrm{i}}\, g(u) \left(\frac{1}{u - \omega - \mathrm{i}\epsilon} - \frac{1}{u - \omega + \mathrm{i}\epsilon} \right) = g(\omega) \tag{3.69}$$

we find

$$g(\omega) = -\mathrm{i}\ \mathrm{Pr}\int \frac{\mathrm{d}u}{\pi}\,\frac{g(u)}{u-\omega}. \tag{3.70}$$

Equation (3.69) follows from the residuum theorem. In Eq. (3.70) the principal value integral is understood. One of various definitions is

$$\mathrm{Pr}\int \frac{\mathrm{d}u}{\pi}\,\frac{g(u)}{u-\omega} = \left(\int_{-\infty}^{\omega-\epsilon} + \int_{\omega+\epsilon}^{\infty}\right)\frac{\mathrm{d}u}{\pi}\,\frac{g(u)}{u-\omega}, \tag{3.71}$$

with $0 < \epsilon \to 0$.

We denote the real part of g by g' and the imaginary part by g'' such that $g(\omega) = g'(\omega) + \mathrm{i}\,g''(\omega)$ holds true, with real valued functions g' and g''. With this we may rewrite Eq. (3.70) as

$$g'(\omega) = \mathrm{Pr}\int \frac{\mathrm{d}u}{\pi}\,\frac{g''(u)}{u-\omega} \text{ and } g''(\omega) = \mathrm{Pr}\int \frac{\mathrm{d}u}{\pi}\,\frac{g'(u)}{\omega-u}. \tag{3.72}$$

If the causal function f is real, its Fourier transform g obeys

$$g^*(\omega) = g(-\omega). \tag{3.73}$$

We then may write

$$g'(\omega) = \mathrm{Pr}\int_0^{\infty} \frac{\mathrm{d}u}{\pi}\,\frac{2u\,g''(u)}{u^2-\omega^2} \tag{3.74}$$

and

$$g''(\omega) = 2\omega\ \mathrm{Pr}\int_0^{\infty} \frac{\mathrm{d}u}{\pi}\,\frac{g'(u)}{\omega^2-u^2}. \tag{3.75}$$

These so called dispersion relations—we shall soon explain why they are called so—are consequences of $f(t) = 0$ for $t < 0$ where f is any real valued causal function and g its Fourier transform. Note that they can be formulated with positive ω and u, i.e., with true frequencies.

3.3.2 Kramers-Kronig Relations

If a system is perturbed by an electric field $E_k = E_k(t,\boldsymbol{x})$, it responds by a polarization $P_j = P_j(t,\boldsymbol{x})$. The Fourier components of the two fields are related, in linear approximation, by $\tilde{P}_j = \epsilon_0 \sum_k \chi_{jk}\tilde{E}_k$, see Eq. (3.60). Because of

$$\chi_{jk}(\omega,\boldsymbol{q}) = \frac{1}{\epsilon_0}\int_0^{\infty} \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega\tau}\int \mathrm{d}^3\xi\ \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{\xi}}\ \Gamma_{jk}(\tau,\boldsymbol{\xi}) \tag{3.76}$$

each component $\chi_{jk}(\omega, \boldsymbol{q})$ is the Fourier transform (with respect to time) of a causal function. Recall Eq. (3.58), i.e.,

$$\Gamma_{jk}(\tau, \boldsymbol{\xi}) = \langle \, \frac{\mathrm{i}}{\hbar} \, [P_j(\tau, \boldsymbol{\xi}), P_k(0)] \, \rangle. \tag{3.77}$$

We therefore may write

$$\chi_{jk}(\omega, \boldsymbol{q}) = -\mathrm{i} \, \mathrm{Pr} \int \frac{\mathrm{d}u}{\pi} \, \frac{\chi_{jk}(u, \boldsymbol{q})}{u - \omega}. \tag{3.78}$$

Let us decompose the susceptibility tensor into a Hermitian (prime) and a anti-Hermitian part (double prime):

$$\chi'_{jk} = \frac{\chi_{jk} + \chi^*_{kj}}{2} \quad \text{and} \quad \chi''_{jk} = \frac{\chi_{jk} - \chi^*_{kj}}{2\mathrm{i}} \tag{3.79}$$

such that $\chi_{jk} = \chi'_{jk} + \mathrm{i}\,\chi''_{jk}$, always at $(\omega, \boldsymbol{q})$. Equation (3.78) become

$$\chi'_{jk}(\omega, \boldsymbol{q}) = \mathrm{Pr} \int \frac{\mathrm{d}u}{\pi} \frac{\chi''_{jk}(u, \boldsymbol{q})}{u - \omega} \tag{3.80}$$

and

$$\chi''_{jk}(\omega, \boldsymbol{q}) = \mathrm{Pr} \int \frac{\mathrm{d}u}{\pi} \frac{\chi'_{jk}(u, \boldsymbol{q})}{\omega - u}. \tag{3.81}$$

The Hermitian contribution χ'_{jk} causes refraction of light and is therefore called the refractive part. χ''_{jk} is called the absorptive or dissipative part of the susceptibility tensor because it describes the absorption of light by the medium under study. The Kramers-Kronig relations (3.80) and (3.81) say that both, the refractive and the absorptive contribution to the susceptibility, necessarily depend non-trivially on the angular frequency ω. Dispersion—the dependency of light propagation on color—is unavoidable. Moreover, there is no refraction without absorption.

Apart from the phenomenon of optical activity, only the susceptibility for $\boldsymbol{q} = 0$ is of interest in optics. In what follows we assume $\boldsymbol{q} = 0$, and we write $\chi_{jk}(\omega)$ for $\chi_{jk}(\omega, 0)$. Because of

$$\Gamma^*_{kj}(\tau, \boldsymbol{\xi}) = \Gamma_{jk}(-\tau, -\boldsymbol{\xi}) \tag{3.82}$$

we conclude

$$\chi^*_{jk}(\omega) = \chi_{kj}(-\omega). \tag{3.83}$$

This is the same as Eq. (3.73) except that now the matrix indexes have to be flipped. Therefore we may rewrite the Kramers-Kronig relations as

$$\chi'_{jk}(\omega) = \mathrm{Pr} \int_0^\infty \frac{\mathrm{d}u}{\pi} \, \frac{2u \, \chi''_{jk}(u)}{u^2 - \omega^2} \tag{3.84}$$

and

$$\chi''_{jk}(\omega) = 2\omega \,\mathrm{Pr} \int_0^\infty \frac{\mathrm{d}u}{\pi} \frac{\chi'_{jk}(u)}{\omega^2 - u^2}. \tag{3.85}$$

Note that the dissipative part $\chi''_{jk}(\omega)$ is an odd function of ω. It vanishes for $\omega = 0$, and the refractive part is well defined for $\omega = 0$. $\epsilon_{jk} = \delta_{jk} + \chi'_{jk}(0)$ is the static permittivity. Also note that the susceptibility—both the refractive and the dissipative part—vanish with $\omega \to \infty$.

3.3.3 *Summary*

A causal function $f = f(t)$ vanishes for $t < 0$. Its Fourier transform $g = g(\omega)$ then fulfills a dispersion relation. The real part of it can be calculated from the imaginary part, and vice versa. We apply these purely mathematical findings to the susceptibility tensor. The Hermitian part, which is responsible for the refraction of light, is intimately related with the anti-Hermitian part which causes absorption. There is no refraction without absorption (at possibly different frequencies), and dispersion is unavoidable. Another consequence of these so-called Kramers-Kronig relations is that the absorptive contribution to the susceptibility vanishes at zero frequency, and both parts vanish with $\omega \to \infty$.

3.4 Fluctuations and Dissipation

We study processes $t \to M_t$ where M is an observable and t denotes time. Expectation values are always with respect to a Gibbs state G. We will discuss auto- and cross-correlations and their Fourier transforms, which are spectral densities. The anti-Hermitian contribution χ''_{jk} of the susceptibility tensor is linearly related with the spectral density matrix S_{jk}. This relation ensures that the anti-Hermitian part of the susceptibility tensor indeed causes dissipation, i.e., loss of field energy. We arrive at a weak formulation of the second law of thermodynamics.

3.4.1 *Wiener-Khinchin Theorem*

Consider a process $M_t = U_{-t} M U_t$ where U_t is the waiting operator[7]

$$U_t = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} tH}. \tag{3.86}$$

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[7] Note that we look upon time within the framework of the Heisenberg picture.

H is the energy observable of the system, its Hamiltonian.

The equilibrium state of the system is

$$G = \mathrm{e}^{(F - H)/k_{\mathrm{B}}T} \tag{3.87}$$

where T denotes its temperature and F, the free energy, serves to normalize G.

Because of

$$\langle GM_t \rangle = \operatorname{tr} GM_t = \operatorname{tr} GU_{-t}MU_t = \operatorname{tr} U_t G U_{-t} M = \operatorname{tr} GM \tag{3.88}$$

the expectation value $\langle M_t \rangle = \langle M \rangle$ does *not* depend on time. Therefore the expectation value of the fluctuation

$$\delta M_t = M_t - \langle M \rangle \tag{3.89}$$

vanishes. However, $\langle (\delta M_t)^2 \rangle$ does not vanish, in general. We generalize this finding and define

$$K(\tau) = \frac{\langle \delta M_{t+\tau}\, \delta M_t \rangle + \langle \delta M_t\, \delta M_{t+\tau} \rangle}{2}. \tag{3.90}$$

The symmetric product $(AB + BA)/2$ of two observables A and B is an observable, and therefore the correlation function $K(\tau)$ is real. It depends on τ only, and not on t, because the expectation value is calculated with respect to the stationary Gibbs state.

Let us now Fourier-decompose the fluctuations,

$$\delta M_t = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t}\, \delta\tilde{M}_\omega, \tag{3.91}$$

or

$$\delta M_{t+\tau} = \int \frac{\mathrm{d}\omega'}{2\pi}\, \mathrm{e}^{\mathrm{i}\omega'(t+\tau)}\, \delta\tilde{M}^\dagger_{\omega'}, \tag{3.92}$$

and insert this into Eq. (3.90). The result contains a factor

$$\int \frac{\mathrm{d}\omega'}{2\pi} \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{\mathrm{i}(\omega' - \omega)t}. \tag{3.93}$$

This factor does *not* depend on t if the rest contributes only for $\omega = \omega'$. In other words,

$$K(\tau) = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{\mathrm{i}\omega\tau}\, S(\omega), \tag{3.94}$$

where $S(\omega)$ is defined by

$$\frac{\langle \delta\tilde{M}^\dagger_{\omega'}\, \delta\tilde{M}_\omega + \delta\tilde{M}_\omega\, \delta\tilde{M}^\dagger_{\omega'} \rangle}{2} = 2\pi\, \delta(\omega' - \omega)\, S(\omega). \tag{3.95}$$

Because of $\langle\, A^\dagger A \,\rangle \geq 0$ we conclude from Eq. (3.95) that the spectral density $S = S(\omega)$ is nowhere negative,

$$S(\omega) \geq 0. \tag{3.96}$$

Equation (3.94) together with Eq. (3.96) is known as Khinchin's or the Wiener-Khinchin theorem. The correlation function $K = K(\tau)$ for fluctuations in a stationary state is the Fourier transform of a non-negative spectral intensity $S = S(\omega)$. Note that $K(0) = \langle\, (\delta M_t)^2 \,\rangle \geq 0$ is compatible with the Wiener-Khinchin theorem.

This was the first step towards the fluctuation-dissipation theorem. The state with respect to which we calculate expectation values had to commute with the Hamiltonian, i.e., it must be stationary. We next specialize to the Gibbs state.

3.4.2 Kubo-Martin-Schwinger Formula

There is a formal similarity between the Gibbs state $G_\beta \propto \mathrm{e}^{-\beta H}$ and the waiting operator $U_\tau = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\tau H}$. Somewhat metaphorically, time t is an imaginary inverse temperature and the inverse temperature β is an imaginary time.

Let us define

$$A_z = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} zH} A\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} zH} \tag{3.97}$$

for a complex number z. We easily may show

$$A_z\, \mathrm{e}^{-\beta H} = \mathrm{e}^{-\beta H}\, \mathrm{e}^{\beta H} A_z\, \mathrm{e}^{-\beta H}, \tag{3.98}$$

or

$$A_z G = G A_{z-\mathrm{i}\hbar\beta}. \tag{3.99}$$

We multiply from the right with B and form the trace. The result is

$$\langle\, B A_z \,\rangle = \langle\, A_{z-\mathrm{i}\hbar\beta} B \,\rangle, \tag{3.100}$$

the famous KMS formula named after Kubo, Martin, and Schwinger. This relation characterizes thermodynamic equilibrium with inverse temperature β. A and B are arbitrary observables, and z is a complex number. A mathematically rigorous formulation is beyond the scope of this book. Note that $\hbar\beta$ is a time.

3.4.3 Callen-Welton Theorem

Assume a time-dependent Hamiltonian $H_t = H - \lambda(t)M$ and a Gibbs state at $t \to -\infty$. The linear response to this perturbation, as felt by the observable M, is given by

$$\langle\, M \,\rangle_t = \langle\, M \,\rangle + \int_0^\infty \mathrm{d}\tau\, \Gamma(\tau)\, \lambda(t-\tau), \tag{3.101}$$

where

$$\Gamma(\tau) = \frac{\mathrm{i}}{\hbar} \langle\, M_\tau\, M - M\, M_\tau \,\rangle \tag{3.102}$$

is the influence function. Note that only fluctuations contribute,

$$\Gamma(\tau) = \frac{\mathrm{i}}{\hbar} \langle\, \delta M_\tau\, \delta M - \delta M\, \delta M_\tau \,\rangle. \tag{3.103}$$

Compare this with the correlation function

$$K(\tau) = \frac{1}{2} \langle\, \delta M_\tau\, \delta M + \delta M\, \delta M_\tau \,\rangle. \tag{3.104}$$

The former expression is the expectation value of a commutator, the latter of an anti-commutator. There should be a relation between Eqs. (3.103) and (3.104).

Define

$$\phi(\tau) = \langle\, \delta M_\tau\, \delta M \,\rangle, \tag{3.105}$$

the Fourier transform of which is

$$\tilde{\phi}(\omega) = \int \mathrm{d}\tau\; \mathrm{e}^{\,\mathrm{i}\omega\tau}\, \phi(\tau). \tag{3.106}$$

By declaring

$$f(z) = \int \frac{\mathrm{d}\omega}{2\pi}\; \mathrm{e}^{-\mathrm{i}\omega z}\, \tilde{\phi}(\omega) \tag{3.107}$$

we analytically continue Eq. (3.105) to complex arguments z.

On the other hand, A_z as defined by Eq. (3.97), gives rise to another function

$$g(z) = \langle\, \delta M_z\, \delta M \,\rangle \tag{3.108}$$

which can be shown to be analytic within a sufficiently broad stripe around the real axis. Since f and g coincide on the real axis, they are equal in the complex plane as well. We may therefore write

$$\langle\, \delta M_\tau\, \delta M \,\rangle = f(\tau) \text{ and } \langle\, \delta M\, \delta M_\tau \,\rangle = f(\tau - \mathrm{i}\hbar\beta). \tag{3.109}$$

After these preparations we may represent the influence function and the correlation function as

$$\Gamma(\tau) = \frac{\mathrm{i}}{\hbar}\,\{f(\tau) - f(\tau - \mathrm{i}\hbar\beta)\} \tag{3.110}$$

and

$$K(\tau) = \frac{1}{2}\{f(\tau) + f(\tau - \mathrm{i}\hbar\beta)\}, \tag{3.111}$$

respectively. Inserting Eq. (3.107) yields

$$\Gamma(\tau) = \frac{\mathrm{i}}{\hbar}\int \frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega\tau}\left\{1 - \mathrm{e}^{-\beta\hbar\omega}\right\}\tilde{\phi}(\omega) \tag{3.112}$$

and

$$K(\tau) = \frac{1}{2}\int \frac{\mathrm{d}\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega\tau}\left\{1 + \mathrm{e}^{-\beta\hbar\omega}\right\}\tilde{\phi}(\omega). \tag{3.113}$$

We can eliminate the unknown function $\tilde{\phi}$ by equating

$$\tilde{\phi}(\omega) = \frac{\hbar}{\mathrm{i}}\,\frac{\tilde{\Gamma}(\omega)}{1 - \mathrm{e}^{-\beta\hbar\omega}} = 2\,\frac{\tilde{K}(\omega)}{1 + \mathrm{e}^{-\beta\hbar\omega}}. \tag{3.114}$$

Note that the Fourier transform of the correlation function is the spectral density $S = S(\omega)$, see Eq. (3.94) with Eq. (3.96). Therefore

$$\tilde{\Gamma}(\omega) = \frac{2\mathrm{i}}{\hbar}\,S(\omega)\,\tanh\frac{\beta\hbar\omega}{2} \tag{3.115}$$

holds true.

However, we are not interested in the Fourier transform of the influence function $\Gamma = \Gamma(\tau)$, but in the (generalized) susceptibility

$$\chi(\omega) = \int \mathrm{d}\tau\,\theta(\tau)\,\mathrm{e}^{\mathrm{i}\omega\tau}\,\Gamma(\tau) = \frac{1}{2\pi\mathrm{i}}\int \mathrm{d}u\,\frac{\tilde{\Gamma}(u)}{u - \omega - \mathrm{i}\epsilon}. \tag{3.116}$$

ϵ in this formula denotes an infinitely small positive number. We easily deduce from this

$$2\mathrm{i}\,\chi''(\omega) = \tilde{\Gamma}(\omega) \tag{3.117}$$

where $\chi''(\omega)$ is the imaginary, or dissipative, contribution to the susceptibility. Equations (3.115) and (3.117) amount to

$$\chi''(\omega) = \frac{1}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)S(\omega). \tag{3.118}$$

This is the famous dissipation-fluctuation theorem as derived by Callen and Welton. $\chi''(\omega)$ describes the dissipation of energy at angular frequency ω, and $S(\omega)$ is the fluctuation spectral density at the same angular frequency. Recall $1/\beta = k_{\mathrm{B}}T$.

Note that Eq. (3.118) reads

$$\chi''(\omega) = \frac{\omega}{2k_{\mathrm{B}}T}\, S(\omega) \tag{3.119}$$

for hight temperatures, or small β. Now $\hbar$ has vanished, we deal with the limiting case of classical statistical mechanics. The limiting case for small temperatures reads

$$\chi''(\omega) = \frac{\operatorname{sgn}(\omega)}{\hbar}\, S(\omega). \tag{3.120}$$

But bear in mind that the spectral density and the dissipative part of the susceptibility depend on temperature because the expectation values in a Gibbs state do so.

3.4.4 Interaction with an Electromagnetic Field

If the Gibbs state is perturbed by more than one external parameter, according to

$$H_t = H - \int \mathrm{d}^3x\, \boldsymbol{P}(\boldsymbol{x}) \cdot \boldsymbol{E}(t, \boldsymbol{x}), \tag{3.121}$$

say, the preceding arguments may easily be adapted.

We not only assume the Gibbs state to be invariant under time translations, but also under space translations. Therefore the expectation value $\langle\, P_j(t, \boldsymbol{x})\,\rangle$, where $P_j(t, \boldsymbol{x}) = U_{-t} P_j(\boldsymbol{x}) U_t$, does not depend on the space and time coordinates. $\delta P_j(t, \boldsymbol{x}) = P_j(t, \boldsymbol{x}) - \langle\, P_j\,\rangle$ is a fluctuation because its expectation value vanishes.

Its space-time correlation functions are

$$K_{jk}(\tau, \boldsymbol{\xi}) = \frac{\langle\, \delta P_j(t+\tau, \boldsymbol{x}+\boldsymbol{\xi})\, \delta P_k(t, \boldsymbol{x}) + \dots\,\rangle}{2}, \tag{3.122}$$

where the dots stand for the preceding factors in reversed order. The Wiener-Khinchin theorem now reads

$$K_{jk}(\tau, \boldsymbol{\xi}) = \int \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{d}^3 q}{(2\pi)^3}\, \mathrm{e}^{\,\mathrm{i}(\omega\tau - \boldsymbol{q}\cdot\boldsymbol{\xi})}\, S_{jk}(\omega, \boldsymbol{q}) \tag{3.123}$$

where S_{jk} is a non-negative matrix, $S \geq 0$.

The subsequent arguments can be translated one-by-one as well.[8] The fluctuation-dissipation theorem no reads

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[8] Note however that the dielectric susceptibility $\chi_{jk}(\omega, \boldsymbol{q})$ is defined by splitting off a factor $1/\epsilon_0$ because of $\boldsymbol{D} = \boldsymbol{P} + \epsilon_0 \boldsymbol{E}$, in usual notation.

$$\chi''_{jk}(\omega, \boldsymbol{q}) = \tanh\left(\frac{\beta\hbar\omega}{2}\right)\frac{S_{jk}(\omega, \boldsymbol{q})}{\hbar\epsilon_0}. \tag{3.124}$$

For each argument $(\omega, \boldsymbol{q})$ the dissipative part χ''_{jk} of the dielectric susceptibility is a non-negative matrix. As we shall show in section *Crystal optics* in Chap. 4, χ''_{jk} is responsible for the attenuation of electromagnetic excitations in passive matter.

By the way, Eq. (3.124) passes the dimension check. The spectral density S is a Fourier transform of the polarization correlation function K which has the dimension of polarization squared. Hence, S/ϵ_0 is an energy times seconds. Divided by $\hbar$, we obtain a dimensionless quantity, namely a susceptibility.

3.4.5 *Summary*

The correlation function $K(\tau)$ for fluctuations $\delta M_{t+\tau}$ and δM_t is the Fourier transform of a positive spectral density $S(\omega)$. This Wiener-Khinchin theorem holds true if the expectation value is calculated for a stationary state. The waiting operator U_t and the Gibbs state G_β are rather similar. Both depend exponentially on the energy H. The Kubo-Martin-Schwinger (KMS) formula is a consequence, in fact, it characterizes the Gibbs state. As it turns out, there is a close relationship between the dissipative part of the susceptibility and the spectral density which characterizes fluctuations. We apply this to the interaction between an electromagnetic field and matter.

3.5 Onsager Relations

The laws of nature do not prefer one direction of time over another, $t \to -t$ is a symmetry. If a movie runs backwards, there should be no means of telling so. The second law of thermodynamics seems to prefer a particular arrow of time, but this is so because we have specified thermodynamic equilibrium conditions in the past which gives rise to irreversible processes with production of entropy.

We will study in this section the consequences of time reversal invariance for susceptibilities and for kinetic coefficients, within the framework of linear response theory. The findings are called Onsager relations. There is, however, a wider field of symmetry relations which apply to a different class of irreversible processes. They refer to fluxes which are driven by gradients of local equilibrium parameters, such as temperature or chemical potentials.

3.5.1 Time Reversal

The system under discussion is represented by a Hilbert space $\mathcal{H}$ of wave functions $\phi = \phi(\boldsymbol{x}_1\sigma_1, \boldsymbol{x}_2\sigma_2, \dots, \boldsymbol{x}_N\sigma_N)$. There are N particles at locations $\boldsymbol{x}_a$ with polarization (spin projection) $\boldsymbol{\sigma}_a$. The wave function must be symmetric upon interchange of equal particles if they are bosons, and antisymmetric for particles of half-integer spin (fermions).[9]

To every linear operator A we assign a time-reversed operator $A^\star$ by

$$(A\phi)^* = A^\star \phi^*. \tag{3.125}$$

As usual in physics, * denotes complex conjugation.

Note that the mapping $A \to A^\star$ is anti-linear in the sense that $A + B$ maps to $A^\star + B^\star$, but zA becomes $z^* A^\star$.

A position operator $\boldsymbol{x}_a$ for particle a amounts to the multiplication of the wave function by the corresponding argument which is real. Therefore $\boldsymbol{x}_a^\star = \boldsymbol{x}_a$ holds true. Linear momentum operators $\boldsymbol{P}_a$ are represented by $-\mathrm{i}\hbar\nabla_a$, therefore $\boldsymbol{P}_a^\star = -\boldsymbol{P}_a$. This is why time reversal is also known as momentum reversal.

Angular momentum operators change their sign upon time reversal as well. The magnetic moment of a particle is proportional to a linear combination of orbital and spin angular momentum both of which change sign. Therefore the magnetization[10] of matter obeys $\boldsymbol{M}^\star(\boldsymbol{x}) = -\boldsymbol{M}(\boldsymbol{x})$. The polarization of matter is the sum of dipole moments $q_a\boldsymbol{x}_a$ per unit volume, it transforms as $\boldsymbol{P}^\star(\boldsymbol{x}) = +\boldsymbol{P}(\boldsymbol{x})$.

Maxwell's equations are invariant with respect to time reversal. We define

- $\boldsymbol{E}^\star(t,\boldsymbol{x}) = +\boldsymbol{E}(-t,\boldsymbol{x})$
- $\boldsymbol{B}^\star(t,\boldsymbol{x}) = -\boldsymbol{B}(-t,\boldsymbol{x})$
- $\varrho^\star(t,\boldsymbol{x}) = +\varrho(-t,\boldsymbol{x})$
- $\boldsymbol{j}^\star(t,\boldsymbol{x}) = -\boldsymbol{j}(-t,\boldsymbol{x})$

in usual notation. It is a simple exercise to show that the time reversed fields obey Maxwell's equation if the original fields do so.

The action of an electromagnetic field on charged particles, as described by the Lorentz force

$$\dot{\boldsymbol{P}} = q\,\{\boldsymbol{E} + \dot{\boldsymbol{x}} \times \boldsymbol{B}\}, \tag{3.126}$$

is compatible with time reversal invariance as well.

The Hamiltonian for ordinary matter is

$$H_\mathrm{m} = \sum_a \frac{\boldsymbol{P}_a^2}{2m_a} + \frac{1}{4\pi\epsilon_0}\sum_{b>a}\frac{q_b\,q_a}{|\boldsymbol{x}_b - \boldsymbol{x}_a|}, \tag{3.127}$$

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[9] Photons, deuterium or helium nuclei are bosons, neutrinos, protons and electrons behave as fermions.

[10] Magnetic moment per unit volume.

where m_a, q_a, $\boldsymbol{x}_a$ and $\boldsymbol{P}_a$ are the mass, charge, location, and linear momentum of particle a, respectively.

Denote by $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{B}}$ an external quasi-static electric and magnetic induction field, respectively. The Hamiltonian for matter in such an external field is

$$H(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}) = H_{\mathrm{m}} - \int \mathrm{d}^3x\, \boldsymbol{\mathcal{E}}(\boldsymbol{x}) \cdot \boldsymbol{P}(\boldsymbol{x}) - \int \mathrm{d}^3x\, \boldsymbol{\mathcal{B}}(\boldsymbol{x}) \cdot \boldsymbol{M}(\boldsymbol{x}). \tag{3.128}$$

From what has been said before we conclude

$$H^{\star}(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}) = H(\boldsymbol{\mathcal{E}},-\boldsymbol{\mathcal{B}}). \tag{3.129}$$

Consequently, a Gibbs state transforms as

$$G^{\star}(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}) = G(\boldsymbol{\mathcal{E}},-\boldsymbol{\mathcal{B}}) \tag{3.130}$$

while the waiting, or time translation, operator obeys

$$U_t^{\star}(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}) = U_{-t}(\boldsymbol{\mathcal{E}},-\boldsymbol{\mathcal{B}}). \tag{3.131}$$

That the magnetic field has to change sign is clear by now. Substituting the time argument t by $-t$ justifies why one speaks of time reversal.

We conclude this section with the following observation. If ϕ is an eigenfunction of A with eigenvalue a, then ϕ^* is an eigenfunction of $A^{\star}$ with eigenvalue a^*. Hence, if M is an observable, so is $M^{\star}$, and if W represents a mixed state, so does $W^{\star}$. Observables are characterized by real eigenvalues. States also have real eigenvalues, moreover, they are probabilities. It is a simple exercise to prove

$$\operatorname{tr} WM = \operatorname{tr} W^{\star}M^{\star}. \tag{3.132}$$

3.5.2 Symmetries for Susceptibilities

We now discuss a Hamiltonian of the form

$$H_t = H(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}}) - \sum_s \lambda_s(t) V_s. \tag{3.133}$$

The response to such a perturbation, as felt by V_r, is

$$\langle V_r \rangle_t = \langle V_r \rangle + \sum_s \int_0^{\infty} \mathrm{d}\tau\, \Gamma_{rs}(\boldsymbol{\mathcal{E}},\boldsymbol{\mathcal{B}};\tau)\, \lambda_s(t-\tau), \tag{3.134}$$

in linear approximation. The matrix of influence functions is given by

$$\Gamma_{rs}(\mathcal{E},\mathcal{B};\tau) = \operatorname{tr} G(\mathcal{E},\mathcal{B})\,\frac{\mathrm{i}}{\hbar}\,[U_{-\tau}(\mathcal{E},\mathcal{B})V_r U_\tau(\mathcal{E},\mathcal{B}),V_s]. \tag{3.135}$$

These response functions depend in a complicated way on the external electric and induction fields $\mathcal{E}$ and $\mathcal{B}$.

With Eq. (3.132) we may write the right hand side as

$$\operatorname{tr} G^\star(\mathcal{E},\mathcal{B})\left\{\frac{\mathrm{i}}{\hbar}\,[U_{-\tau}(\mathcal{E},\mathcal{B})V_r U_\tau(\mathcal{E},\mathcal{B}),V_s]\right\}^\star, \tag{3.136}$$

which equals

$$-\operatorname{tr} G(\mathcal{E},-\mathcal{B})\,\frac{\mathrm{i}}{\hbar}\,[U_\tau(\mathcal{E},-\mathcal{B})V_r^\star U_{-\tau}(\mathcal{E},-\mathcal{B}),V_s^\star] \tag{3.137}$$

or

$$\operatorname{tr} G(\mathcal{E},-\mathcal{B})\,\frac{\mathrm{i}}{\hbar}\,[V_s^\star,U_\tau(\mathcal{E},-\mathcal{B})V_r^\star U_{-\tau}(\mathcal{E},-\mathcal{B})]. \tag{3.138}$$

Expression (3.138) may be time-shifted by $-\tau$. It then reads

$$\operatorname{tr} G(\mathcal{E},-\mathcal{B})\,\frac{\mathrm{i}}{\hbar}\,[U_{-\tau}(\mathcal{E},-\mathcal{B})V_s^\star U_\tau(\mathcal{E},-\mathcal{B}),V_r^\star]. \tag{3.139}$$

We now assume that the observables V_r have a definite parity under time reversal:

$$V_r^\star = \eta_r V_r. \tag{3.140}$$

The time-reversal parity is either $+1$ or -1, because of $(A^\star)^\star = A$.

The result of all this is

$$\Gamma_{rs}(\mathcal{E},\mathcal{B};\tau) = \eta_r\,\eta_s\,\Gamma_{sr}(\mathcal{E},-\mathcal{B};\tau). \tag{3.141}$$

By multiplying Eq. (3.141) with the step function $\theta(\tau)$ and Fourier transforming, we arrive at symmetry relations for susceptibilities:

$$\chi_{rs}(\mathcal{E},\mathcal{B};\omega) = \eta_r\,\eta_s\,\chi_{sr}(\mathcal{E},-\mathcal{B};\omega). \tag{3.142}$$

They should be read as follows. Perturbing matter by V_s and probing the effect by V_r is the same as perturbing by V_s and monitoring V_r. However, this is true only if the direction of an external induction field is reversed as well. If the time reversal parities of V_r and V_s are different, a minus sign shows up. Note that the symmetry rules (3.142) apply both to the Hermitian contribution $\chi'_{rs}(\mathcal{E},\mathcal{B};\omega)$ and to the absorptive part $\chi''_{rs}(\mathcal{E},\mathcal{B};\omega)$.

We call Eq. (3.142) Onsager relations although they were not derived by him within the framework of linear response theory. He discussed irreversible processes of a more general nature. There are generalized forces and generalized fluxes. In lowest order, fluxes are linearly related with forces. The corresponding matrix of kinetic coefficients, which describes direct and cross effects, should be symmetric. We will address this in the next subsection for external parameters as driving forces. A further section is dedicated to driving forces which are gradients of equilibrium parameters, such as temperature or chemical potentials.

3.5.3 Symmetries for Conductivities

Let us define the flux of V by

$$J = \dot{V} = \frac{\mathrm{i}}{\hbar}\,[H, V], \tag{3.143}$$

where H is the Hamiltonian of the system under discussion. For example, if $V = \boldsymbol{P}(\boldsymbol{x})$ stands for the electric polarization, then

$$\boldsymbol{J}(\boldsymbol{x}) = \dot{\boldsymbol{P}}(\boldsymbol{x}) = \sum_a q_a \dot{\boldsymbol{x}}_a \delta^3(\boldsymbol{x}_a - \boldsymbol{x}) \tag{3.144}$$

are the three components of the electric current density.

Now, the expectation value of a commutator vanishes, there are no fluxes in thermal equilibrium.[11] Therefore, $\langle\, J \,\rangle = 0$. With

$$V(t) = U_{-t}\, V\, U_t \tag{3.145}$$

we conclude

$$J(t) = \dot{V}(t) = \frac{\mathrm{d}}{\mathrm{d}t} V(t). \tag{3.146}$$

Note that the dot above a symbol for an observable denotes its rate of change with respect to time, in the language of the Schrödinger picture. In the Heisenberg picture, where observables—not states—depend on time, the same dot refers to the derivative with respect to time.

Having said this, we may work out

$$J_r(t) = \langle\, J_r \,\rangle_t = \sum_s \int_0^\infty \mathrm{d}\tau\; \dot{\varGamma}_{rs}(\tau)\, \lambda_s(t-\tau). \tag{3.147}$$

We refer to the perturbation as described by Eq. (3.133), and we have dropped, for the moment, the quasi-static external fields $\boldsymbol{\mathcal{E}}$ as well as $\boldsymbol{\mathcal{B}}$. The influence functions $\dot{\varGamma}_{rs}$ here are the time derivatives of the expressions given by Eq. (3.135). By Fourier

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[11] Super-conductivity or super-fluidity do not fit into this framework.

transforming Eq. (3.147) we arrive at

$$\tilde{J}_r(\omega) = \sum_s \sigma_{rs}\, \tilde{\lambda}_s(\omega) \tag{3.148}$$

with the conductivity matrix

$$\sigma_{rs}(\omega) = \int_0^\infty \mathrm{d}\tau\ \mathrm{e}^{\,\mathrm{i}\omega\tau}\, \dot{\Gamma}_{rs}(\tau). \tag{3.149}$$

We differentiate relation (3.141) with respect to time, multiply with the step function $\theta = \theta(\tau)$ and perform the Fourier transform. We obtain the following Onsager relations for conductivities:

$$\sigma_{rs}(\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}; \omega) = \eta_r \eta_s\, \sigma_{sr}(\boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}; \omega). \tag{3.150}$$

We shall discuss, in section *Ohm's law and Hall effect*, an example of an Onsager relation for conductivities.

3.5.4 Symmetries for Kinetic Coefficients

Onsager's relations in a more general sense include all sorts of driving forces, not only perturbations by varying external parameters.[12]

Just look at the expression (1.124) for the entropy production rate per unit volume. It may be written as

$$\pi(S) = \sum_a \Phi_a X_a, \tag{3.151}$$

where the Φ_a are fluxes and the X_a play the role of driving forces. Normally, in global thermodynamic equilibrium, the forces as well as the fluxes vanish.

The contribution of heat conduction may serve as an example. It reads

$$\pi(S) = \boldsymbol{J}^{\mathrm{u}} \cdot \nabla \frac{1}{T} + \cdots \tag{3.152}$$

In global thermodynamic equilibrium the temperature field would be constant and there is no gradient of the temperature field. However, if there are temperature

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[12] Every system has an environment. There are actions of the environment on the system such that the re-action of the system on the environment can be neglected. A parameter describing such a one-sided action of the environment on a system is called external. Just think of a static electric field $\boldsymbol{\mathcal{E}}$ produced by a plate capacitor the voltage of which is kept constant.

gradients, they will drive heat[13] and possibly other currents. In the current context we call $\boldsymbol{J}^{\mathrm{u}}$ a flux and $\nabla(1/T)$ a driving force.

If the perturbations of the thermodynamic equilibrium are small, or if we are close to equilibrium, the following simple argument is rather plausible. Without driving forces X_a there should be no fluxes. If the driving forces are small, the fluxes should be small es well. Therefore, close to thermodynamic equilibriums we expect a linear relationship between fluxes and driving forces,

$$\Phi_b = \sum_a K_{ba} X_a. \tag{3.153}$$

In Chap. 2 we have discussed quite a few examples.

The elements of the matrix K in Eq. (3.153) are kinetic coefficients. In fact, the matrix K of kinetic coefficients should have been defined by

$$K_{ba} = \frac{\partial^2 \pi(S)}{\partial X_b \partial X_a}. \tag{3.154}$$

It is therefore symmetric. Supporting arguments are:

- Any real valued matrix K may be split into a symmetric and an anti-symmetric part. The latter would not contribute to entropy production and should vanish.
- $\boldsymbol{X} = L\boldsymbol{X}'$ defines new driving forces as linear combinations of old ones.[14] In order to guarantee Eq. (3.151), namely $\pi(S) = \boldsymbol{\Phi}^{\dagger}\boldsymbol{X}$, we have to set $\boldsymbol{\Phi}' = L^{\dagger}\boldsymbol{\Phi}$. Now, $\boldsymbol{\Phi}' = L^{\dagger}\boldsymbol{\Phi} = L^{\dagger}K\boldsymbol{X} = L^{\dagger}KL\boldsymbol{X}'$. The new matrix of kinetic coefficients is $K' = L^{\dagger}KL$. It is symmetric if K is. Onsager's relations are stable against linear re-definitions of driving forces.
- If the driving force is an external parameter, such as an electric field strength, we have already demonstrated Onsager's theorem.

Onsager's very general statement on the matrix of kinetic coefficients reads as follows:

$$K_{ba}(\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}) = K_{ab}(\boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}). \tag{3.155}$$

We will not try to prove it because this would open up a new field, that of non-equilibrium thermodynamics. Onsager's arguments for his theorem rely on the ingredients which we have referred to in the preceding sections: first order response to perturbations of global equilibrium, and symmetry with respect to time reversal.

The matrix K of kinetic coefficients is not only symmetric, but also positive, as required by the second law of thermodynamics. Note that with K the matrix $K' = LKL^{\dagger}$ is positive as well.

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[13] The heat current density $\boldsymbol{J}^{\mathrm{u}}$ is nothing else but the conduction part of the internal energy current density.

[14] The square matrix L must not be singular.

Temperature gradients, for example, may drive heat currents as well as electric currents. Likewise, the gradient of an electrochemical potential will generate an electric as well as a heat current. The cross kinetic coefficients are related by Onsager's relations. We shall discuss this in greater detail in the example section on *Thomson, Seebeck and Peltier Effect*.

3.5.5 Summary

Small perturbations of the thermal equilibrium state of a system will lead to small non-equilibrium effects. Such effects are described by susceptibilities, by conductivities, and by kinetic coefficients. All of them are matrices the first index of which enumerates the sensor and the second index enumerates the driver. The effect of driver a on sensor b is the same as the effect of driver b on sensor a. However, this is true only if interchanging a and b is accompanied by reversing an external induction field.

Chapter 4
Examples

This is a collection of short articles on various aspects of continuum physics. They are intended to familiarize the reader with applications, in contrast to the more formal approach of the preceding chapters. The collection is neither complete nor systematic, we therefore simply order the articles alphabetically by their titles. The examples are standard problems in

- Acoustics
  - Sound in air
  - Bulk and surface waves in solids
  - Vibrating strings and membranes
- Optics
  - Crystal optics
  - Pockels effect
  - Faraday effect
  - Optical activity
  - Metamaterials
  - Dielectric planar waveguides
  - Surface dielectric waveguide
- Aero- and hydrodynamics
  - Archimedes' principle
  - Bernoulli's law
  - Hagen-Poiseuille law
  - Stoke's law
  - Reynold's number
  - White dwarfs

P. Hertel, *Continuum Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-642-29500-3_4,

- Elasticity
  - Elasticity moduli
  - Beam bending and buckling
  - Stress concentration
- Heat conduction and diffusion
  - Fourier's solution of a heat conduction problem
  - Ice layer
  - Reactions and diffusion
- Charge conduction
  - Ohm's law and Hall effect
  - Thomson, Seebeck and Peltier effect
- Fluctuations
  - Brownian motion
  - Thermal noise in a resistor

One could also group the articles by the type of differential equation to be solved: ordinary or partial, the latter elliptical, parabolic or hyperbolic, or of Stefan type. Other likewise sensible grouping principles would be by substance (fluid, solid, conducting and so forth) or by transported quantity (particles, electric charge, momentum, internal energy, electromagnetic field energy).

However, the world, even if looked upon by a physicist, cannot be categorized convincingly into compartments, and so we order our topics very pragmatically, namely alphabetically by title. I tried to cover the basics of what is considered to be continuum physics and illustrate it by 27 articles. These examples are chosen such that as many aspects as possible are touched.

One article is found here because there is no better place, a discussion on *Natural units*, also known as atomic units. After all, the properties of normal matter are described by the quantum theory of electrostatic interaction. Therefore, any sensible result is a number multiplying a product of powers of $\hbar$, e, m and $4\pi\epsilon_0$, that is, Plank's constant, the elementary charge, the electron mass and the constant showing up in Coulomb's force law.

Occasionally we cite values of physical constants. They are taken mostly from the tables of Kaye and Laby [5]. These are concise and complete enough for our purpose. Moreover, they are published by the National Physical Laboratory in the World Wide Web (http://www.kayelaby.npl.co.uk/).

4.1 Archimedes' Principle

Archimedes of Syracuse, who lived in the Greek colony on Sicily, was a genius mathematician and physicist. Among other mathematical laws and practical applications he found out that the buoyancy of a body in water is equal to the weight of the displaced liquid. With it he could show that the king's crown did not consist of gold because it displaced more water than an equally heavy bar of gold. This made him famous.

It is a seemingly simple task to prove Archimedes' principle. However, a general formal derivation is either wrong or restricted to incompressible fluids, such as water. Nevertheless, the principle is also applied to calculate the buoyant force of balloons in air which is highly compressible. Most elementary text books avoid this topic.

A fluid is described by the momentum balance equation (2.2):

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\partial_k p + f_k + \partial_i T''_{ik}. \tag{4.1}$$

The reversible part of the stress tensor is $T'_{ik} = -p\delta_{ik}$, it does not support shear forces. Recall that ϱ is the mass density, v_k the velocity field, p the pressure, and T''_{ik} describes friction. f_k is the external force per unit volume.

We look for a static solution. The liquid does not flow. Therefore the velocity field vanishes and there is no friction. Thus we have to solve

$$-\partial_k p + f_k = 0 \tag{4.2}$$

with

$$f_1 = f_2 = 0 \text{ and } f_3 = -\varrho g, \tag{4.3}$$

where $g = 9.81\ \mathrm{m\,s^{-1}}$ is the acceleration constant at the earth's surface. Increasing x means upwards.

We ask for the force exercised by the fluid on a totally immersed rigid body occupying the volume[1] $\mathcal{V}$. It is given by the surface integral

$$F_k = \int_{\partial\mathcal{V}} \mathrm{d}A_i T'_{ik} = -\int_{\partial\mathcal{V}} \mathrm{d}A_k p. \tag{4.4}$$

4.1.1 Erroneous Reasoning

One is tempted to write

$$F_k = -\int_{\partial\mathcal{V}} \mathrm{d}A_k p = -\int_{\mathcal{V}} \mathrm{d}V\, \partial_k p = g\delta_{3k} \int_{\mathcal{V}} \mathrm{d}V\, \varrho = gM\delta_{3k}. \tag{4.5}$$

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[1] There is no overall accepted terminology which distinguishes between a three-dimensional manifold $\mathcal{V}$, a volume, and its content V, likewise called volume.

M is the mass of the displaced fluid, gM its weight, and the buoyancy is directed opposite to the gravitational force. So far, so good.

However, M is an integral over the interior of the rigid body, so what is the meaning of ϱ there? Archimedes speaks of the mass of the *displaced* fluid, hence ϱ stands for the mass of the fluid in the absence of an immersed body, or what? All this makes sense only if the mass density is a constant, if the fluid is incompressible. Then the mass density outside $\mathcal{V}$ and inside $\mathcal{V}$—if the volume were flooded—are the same. However, we did not require that the mass density is constant.

Apart from ambiguities of interpretation, there is a mathematical glitch in Eq. (4.5). The Gauss theorem was applied which makes sense only for smooth (continuously differentiable) fields. The mass density certainly is not differentiable, it will jump at the surface $\partial\mathcal{V}$. The result (4.5) seems to be all right, but the way towards it is not.

4.1.2 Incompressible Fluid

If the fluid is supposed to be incompressible, which is a very good approximation for water, the proof of Archimedes' principle is simple. Recall that an incompressible fluid is characterized by the material equation ϱ = const or by $\partial_k \varrho = 0$.

Equation (4.3) can be reformulated as

$$f_k = -\varrho \partial_k \phi_{\mathrm{g}} = -\partial_k \varrho \phi_{\mathrm{g}} \text{ where } \phi_{\mathrm{g}}(\boldsymbol{x}) = g x_3. \tag{4.6}$$

Equation (4.2) now reads

$$\partial_k (p + \varrho g x_3) = 0, \tag{4.7}$$

which implies

$$p(\boldsymbol{x}) = p_0 - \varrho g x_3 \tag{4.8}$$

and

$$F_k = \varrho g \int_{\partial\mathcal{V}} \mathrm{d}A_k \, x_3. \tag{4.9}$$

This time a continuously differentiable field is to be integrated, and we easily work out

$$\int_{\partial\mathcal{V}} \mathrm{d}A_k \, x_3 = \int_{\mathcal{V}} \mathrm{d}V \, \partial_k x_3 = \delta_{3k} V, \tag{4.10}$$

where V stands for the volume of the immersed body. Equations (4.9) and (4.10) say $F_1 = F_2 = 0$ and $F_3 = g\varrho V$. This is Archimedes' principle.

4.1.3 Compressible Fluid

We want to find out whether Archimedes' principle is valid for air as well which we model as an ideal gas:

$$p = \frac{\varrho}{M} RT. \tag{4.11}$$

M is the molar mass and $R = 8.314\,\mathrm{J\,K^{-1}\,mol^{-1}}$ the universal gas constant, see Eq. (2.10). The molar mass for dry air is $0.02897\,\mathrm{kg\,mol^{-1}}$.

We have to solve the equation for hydrostatic equilibrium

$$p' = -g\varrho = -\frac{gM}{RT} p, \tag{4.12}$$

where the prime denotes differentiation with respect to height x_3. For a model atmosphere with constant temperature the solution is

$$p(\boldsymbol{x}) = p_0\, \mathrm{e}^{-\kappa x_3} \text{ where } \kappa = \frac{gM}{RT}, \tag{4.13}$$

the barometric formula. Although it does not describe the atmosphere well, it may serve to derive Archimedes' buoyancy formula and corrections. We will discuss a far more realistic model of the atmosphere in another article.

We have to work out the following integral:

$$F_k = -\int_{\partial\mathcal{V}} \mathrm{d}A_k\, p = -\int_{\mathcal{V}} \mathrm{d}V\, \partial_k\, p. \tag{4.14}$$

Assume that the rigid body is positioned at $\boldsymbol{x} = \bar{\boldsymbol{x}}$. We introduce local, or center of buoyancy coordinates $\boldsymbol{\xi}$ by $\boldsymbol{x} = \bar{\boldsymbol{x}} + \boldsymbol{\xi}$ in such a way that

$$\int_{\mathcal{V}} \mathrm{d}^3\xi\, \xi_k = 0. \tag{4.15}$$

With this one may write

$$F_k = -p(\bar{\boldsymbol{x}}) \int_{\mathcal{V}} \mathrm{d}^3\xi\, \partial_k\, \mathrm{e}^{-\kappa\xi_3}, \tag{4.16}$$

therefore

$$F_k = \kappa p(\bar{\boldsymbol{x}})\delta_{3k} \int_{\mathcal{V}} \mathrm{d}^3\xi \left(1 - \kappa\xi_3 + \frac{\kappa^2}{2}\xi_3^2 + \dots\right). \tag{4.17}$$

The first term gives

$$F_3 = \kappa p(\bar{\boldsymbol{x}})V = g\varrho(\bar{\boldsymbol{x}})V, \tag{4.18}$$

as stated by Archimedes' principle. The second term vanishes. The third term provides a correction,

$$F_3 = g\varrho(\bar{\boldsymbol{x}})V \left\{ 1 + \frac{\kappa^2}{2V} \int_{\mathcal{V}} \mathrm{d}^3\xi \, \xi_3^2 + \dots \right\}. \tag{4.19}$$

If the object has a size ℓ, the correction will be of order $\kappa^2 \ell^2$. With $1/\kappa = 8.76\,\mathrm{km}$ for $T = 300\,\mathrm{K}$, the correction is tiny and can safely be neglected. Other models of the atmosphere allow a similar observation.

We conclude that Archimedes' principle holds true both for incompressible and highly compressible fluids, such as water or air.

4.2 Beam Bending and Buckling

A beam,[2] or member, or rod, is a long body of usually constant cross section to be used in machines and structures of all kind. It serves to guide momentum currents, i.e., transmit mechanical forces. Let it be wood, reinforced concrete or steel: beams are used to build houses and their roofs, from huts to skyscrapers, you find them in cranes, bridges, power line masts, sailing boats, airplanes, ships and cars, and so on. The theory of elastic beams, as developed by Euler and Bernoulli, provides a tool for the analysis of stresses within the beam for given load and boundary conditions, it is the key element of structural engineering. The aim of this short article is to embed beam theory into the general framework of continuum physics. We follow the line of arguments of Landau and Lifshitz [6].

A straight beam, when being pressed upon by a force, will deform accordingly, remaining straight. However, if the force exceeds a certain limit, the beam tends to bend and finally to buckle and break. We will discuss this phenomenon in more detail, also because it is an example of spontaneous symmetry breaking.

4.2.1 Beam Theory

The undeformed beam is a cylinder of cross section Ω and length ℓ. Its axis is parameterized by z, the cross section by x, y such that x, y, z form a Cartesian coordinate system. The origin of the cross section coordinates is chosen such that

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[2] Not to be confused with a beam of light or particles.

$$\int_\Omega \mathrm{d}A\, x = \int_\Omega \mathrm{d}A\, y = 0. \tag{4.20}$$

$\mathrm{d}A = \mathrm{d}x\,\mathrm{d}y$ is the area element. The first momenta will vanish. The second momenta are

$$I_x = \int_\Omega \mathrm{d}A\, y^2 \text{ and } I_y = \int_\Omega \mathrm{d}A\, x^2. \tag{4.21}$$

The x, y coordinate axes shall be chosen such that the integral of xy over the cross section vanishes which is always possible. By Eq. (4.20) and the latter requirement we have defined the cross section coordinates uniquely.[3] The undeformed beam is the region $x, y \in \Omega$ and $z \in [0, \ell]$.

A rectangular beam, for example, is described by $x \in [-a/2, a/2]$ and $y \in [-b/2, b/2]$. Obviously the first momenta vanish. The second momenta are

$$I_x = \frac{1}{12}a^3 b \text{ and } I_y = \frac{1}{12}ab^3, \tag{4.22}$$

while the integral of xy vanishes, as it should.

The line $(x, y, z) = (0, 0, z)$ is the beam axis. If the beam is weakly bent, the axis remains unstressed, as we shall see. Therefore, the beam axis and the so called neutral fiber are one and the same.

Bending Momentum and Elastic Energy

Let us discuss a short piece of the beam at z. Denote by $R = R(z)$ the radius of curvature. We assume bending in the x, z plane. Note that R refers to the beam axis. The radius of curvature for position x is $R + x$. If follows that the distance $\mathrm{d}z$ on the beam axis becomes, after bending, the distance

$$\mathrm{d}z' = \frac{R + x}{R}\mathrm{d}z = \left(1 + \frac{x}{R}\right)\mathrm{d}z, \tag{4.23}$$

because tangential lengths change by the ratio $R(x)/R(0) = (R + x)/R$. The relative change by bending is

$$S_{zz} = \frac{\mathrm{d}z'}{\mathrm{d}z} = \frac{x}{R}. \tag{4.24}$$

As announced before, the longitudinal strain vanishes at the beam axis. It varies linearly with the x coordinate multiplied by $\kappa = R^{-1}$ which measures curvature.

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[3] Up to interchanging x with y or $x \to -x$ or $y \to -y$ or both.

The stress corresponding to Eq. (4.24) is

$$T_{zz} = E\frac{x}{R}. \tag{4.25}$$

This justifies our choice of the beam axis according to Eq. (4.20): it suffers no stress upon bending.

The components $T_{xx}, T_{xy} = T_{yx}$ and T_{yy} vanish at the boundary $\partial\Omega$. Because the radius of curvature is large with respect to x, y within the beam cross section, the boundary values are to be interpolated linearly. Hence, $T_{xx}, T_{xy} = T_{yx}$ and T_{yy} vanish everywhere, not only at the boundary. A similar argument leads to $T_{xz} = T_{zx} = T_{yz} = T_{zy} = 0$. The stress tensor has no other non-vanishing element but T_{zz}. The corresponding strain tensor is

$$S_{jk} = \frac{\partial_j u_k + \partial_k u_j}{2} = \begin{pmatrix} -\nu & 0 & 0 \\ 0 & -\nu & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{x}{R}, \tag{4.26}$$

according to Hooke's law. ν is Poisson's ratio. It can be integrated to a displacement field $\boldsymbol{u}(x, y, z)$, therefore, the compatibility conditions for the stress tensor are met.

The torque, or bending moment, exercised on the cross section is

$$M_y = \int_\Omega \mathrm{d}A\, x T_{zz} = \frac{E}{R} I_y, \tag{4.27}$$

where we have used Eqs. (4.25) and (4.21). Since bending takes place in the x, z plane, the analogous bending moment M_x vanishes.

Elastic Energy

Generally, the contribution of deformation to the free energy F is described by

$$\mathrm{d}F = \int \mathrm{d}V\, T_{jk} \mathrm{d}S_{jk}, \tag{4.28}$$

which, for a linear medium, can be integrated to

$$F_{\mathrm{el}} = \frac{1}{2} \int \mathrm{d}V\, T_{jk} S_{jk}. \tag{4.29}$$

In our case the elastic energy per unit beam length is

$$\frac{\mathrm{d}F_{\mathrm{bnd}}}{\mathrm{d}z} = \frac{E}{2R^2} \int_\Omega \mathrm{d}A\, x^2 = \frac{EI_y}{2R^2} = \frac{M_y^2}{2EI_y}. \tag{4.30}$$

Note that E and I_y are constants while R or M_y depend on z.

Before bending, the neutral fiber, or beam axis, was the curve $z \to (0, 0, z)$. After bending, the same neutral fiber is described by

$$z \to \boldsymbol{\xi}(s) = (X(z), Y(z), z). \tag{4.31}$$

Let us again specialize to bending in the x, z plane, i.e., to $Y(z) = 0$. The tangent vector is

$$\boldsymbol{t}(z) = \frac{\mathrm{d}\boldsymbol{\xi}(z)}{\mathrm{d}z} = \begin{pmatrix} X'(z) \\ 0 \\ 1 \end{pmatrix}. \tag{4.32}$$

It is almost a unit vector because

$$|\boldsymbol{t}| = \sqrt{1 + X'^2} \approx 1, \tag{4.33}$$

since we assumed that the beam is bent just weakly. Put otherwise, the arclength increment $\mathrm{d}s$ and $\mathrm{d}z$ are nearly the same,

$$\mathrm{d}z = \sqrt{1 + X'^2}\mathrm{d}s = \mathrm{d}s + \frac{1}{2}X'^2\mathrm{d}s \approx \mathrm{d}s. \tag{4.34}$$

Consequently, the radius of curvature is determined by

$$\frac{1}{R(z)} = \kappa(z) = \pm \left| \frac{\mathrm{d}\boldsymbol{t}(z)}{\mathrm{d}z} \right| = X''(z). \tag{4.35}$$

The plus or minus sign takes into account that the center of the curvature circle may be to the right or left of the curve. The elastic energy can thus be expressed as

$$F_{\text{bnd}} = \frac{E}{2} \int_0^\ell \mathrm{d}z \, \{ I_y X''(z)^2 + I_x Y''(z)^2 \}, \tag{4.36}$$

for simultaneous bending in the x, z and in the y, z planes.

External Forces

There may be external forces acting on the beam, perpendicularly or longitudinally. A perpendicular external force per unit length with components $K_x = K_x(z)$ and $K_y = K_y(z)$ contributes to the free energy with

$$F_{\text{prp}} = -\int_0^\ell \mathrm{d}z \, \{ K_x(z)X(z) + K_y(z)Y(z) \}. \tag{4.37}$$

The work done by the longitudinal force T is $T\Delta\ell$. The latter factor, the amount by which the beam is stretched, is given by

$$\Delta\ell = \int_0^\ell \mathrm{d}z\,\frac{\mathrm{d}z-\mathrm{d}s}{\mathrm{d}z} = \frac{1}{2}\int_0^\ell \mathrm{d}z\,\frac{1}{2}\left\{X'(z)^2+Y'(z)^2\right\}. \tag{4.38}$$

Hence the contribution of a longitudinal force T to the free energy is

$$F_{\mathrm{lon}} = \frac{T}{2}\int_0^\ell \mathrm{d}z\,\left\{X'(z)^2+Y'(z)^2\right\}. \tag{4.39}$$

T here stands for tension, not for stress or temperature.

4.2.2 Equilibrium

At the equilibrium configuration the free energy of a system attains a minimum. In our case, the variation δF has to vanish for arbitrary small deviations δX and δY from their equilibrium value. δX and δY should be compatible with the boundary conditions of the special problem under study. On either side of the beam, at $z=0$ and at $z=\ell$, one of three boundary conditions shall be realized:

- Free: $X''=0$ and $X'''=0$,
- Fixed: $X=0$ and $X''=0$,
- Clamped: $X=0$ and $X'=0$,

and analogously for Y. For example, when partially integrating

$$\delta\int_0^\ell \mathrm{d}z\,X''^2 = 2\int_0^\ell \mathrm{d}z X''\delta X'' = -2\int_0^\ell \mathrm{d}z\,X'''\delta X', \tag{4.40}$$

the terms $X''(\ell)\delta X'(\ell)$ and $X''(0)\delta X'(0)$ vanish for free, fixed and clamped boundary conditions. Partially integrating once more gives

$$\delta\int_0^\ell \mathrm{d}z\,X''^2 = 2\int_0^\ell \mathrm{d}z\,X''''\delta X, \tag{4.41}$$

because $X'''\delta X$ vanishes for $x=0$ and $x=\ell$ if the beam there is free, fixed, or clamped.

For a beam bent in the x,z plane, the free energy to minimize is

$$F = \int_0^\ell \mathrm{d}z\,\left\{\frac{EI_y}{2}X''(z)^2 - K_x(z)X(z) + \frac{T}{2}X'(z)^2\right\}. \tag{4.42}$$

With one of the above mentioned boundary conditions for $z = 0$ and one of them for $z = \ell$ we find

$$\delta F = \int_0^\ell \mathrm{d}z \left\{ EI_y X''''(z) - K_x - TX''(x) \right\} \delta X = 0, \tag{4.43}$$

which results in

$$EI_y X''''(z) = TX''(z) + K_x(z), \tag{4.44}$$

and, by an identical line of arguments, in

$$EI_x Y''''(z) = TY''(z) + K_y(z). \tag{4.45}$$

Recall that E is Young's elasticity module. I_y and I_x are moments as defined by Eq. (4.21). K_x and K_y denote external perpendicular forces per unit length in x or y direction. T is a force in longitudinal direction, usually drawing ($T > 0$) or pressing ($T < 0$) at the front end $z = \ell$. The neutral fiber of the undeformed bar, parameterized by z, is deflected by $X(z)$ and $Y(z)$ in x and y direction, respectively. Equations (4.44) and (4.45) are approximations for weakly bent slender beams.

4.2.3 An Example

Think about a cantilever of length ℓ. It is clamped at $z = 0$, free at $z = \ell$ and bent by its own weight. We have to solve

$$EI_y X''''(z) = K_x \text{ where } K_x = -g\varrho A. \tag{4.46}$$

g is the acceleration due to gravity, ϱ denotes mass density, and A is the cantilever's cross section area. The boundary conditions to be observed are

$$X(0) = 0\,,\ X'(0) = 0\,,\ X''(\ell) = 0 \text{ and } X'''(\ell) = 0. \tag{4.47}$$

We try a polynomial of degree four such that the fourth derivative is a constant. The boundary conditions at $z = 0$ and the differential equation suggest

$$X(z) = -\frac{g\varrho A}{24EI_y} \left\{ z^4 + a\ell z^3 + b\ell^2 z^2 \right\}. \tag{4.48}$$

The boundary conditions at $z = \ell$ require $a = -4$ and $b = 6$. The solution therefore reads

$$X(z) = -\frac{g\varrho A}{24EI_y} \left\{ z^4 - 4\ell z^3 + 6\ell^2 z^2 \right\}. \tag{4.49}$$

With $\xi = z/\ell$ we may rewrite this into

$$X(z) = -\frac{g\varrho A\ell^4}{8EI_y}\left\{\frac{1}{3}\xi^2 - \frac{4}{3}\xi + 2\right\}\xi^2. \tag{4.50}$$

The expression in ξ increases monotonically from zero to one, therefore, the factor in front of the curly bracket is the maximal cantilever deflection.

4.2.4 Buckling Instability

We now discuss a thin rod without lateral forces under pressure. Denote by $F = -T$ the longitudinal compressing force exerted on the front end at $x = \ell$. One has to solve

$$EI_y X'''' + FX'' = 0. \tag{4.51}$$

We demand the rod to be fixed (but not clamped) at both ends, i.e.,

$$X(0) = X(\ell) = 0 \text{ and } X''(0) = X''(\ell) = 0. \tag{4.52}$$

The solution of Eq. (4.51) is a linear combination of its four fundamental solutions, namely

$$X(z) = a + bz + c\cos qz + d\sin qz \text{ with } q = \sqrt{\frac{F}{EI_y}}. \tag{4.53}$$

Now, $X''(0) = 0$ says $c = 0$. $X(0) = 0$ requires $a = 0$. $X''(\ell) = 0$ may be satisfied either with $d = 0$ or with $q\ell = n\pi$ for $n = 1, 2, \dots$ The boundary condition $X(\ell) = 0$ makes b to vanish.

Define the critical force by

$$F_{\mathrm{cr}} = \frac{\pi^2 EI_y}{\ell^2}. \tag{4.54}$$

If $F < F_{\mathrm{cr}}$, the second alternative for satisfying $X''(\ell) = 0$ is impossible, and we have to choose $d = 0$. Our problem then has the solution $X(z) = 0$. The rod can stand the load and does not bend. This is what we expect from a pillar: it carries its load, gets a bit shorter and broader, but remains straight.

If $F = F_{\mathrm{cr}}$, the solution is

$$X(z) = d\sin qz \text{ with } q = \sqrt{\frac{F_{\mathrm{cr}}}{EI_y}}, \tag{4.55}$$

for arbitrary d.

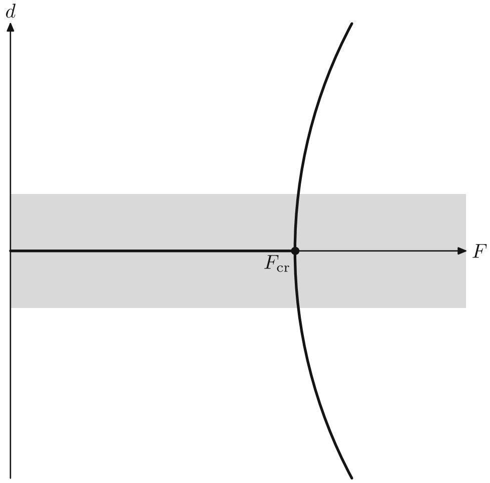

Fig. 4.1 A thin rod with fixed (not clamped) boundary conditions is compressed by a longitudinal force F. The deflection is described by $X(z) = d\,\sin(\pi z/\ell)$. As long as the force is smaller than the critical value F_{cr} the rod remains straight, $d = 0$. For larger forces, d increases rapidly and leading finally to buckling. Outside the *shaded region* the approximation of small bending is no longer applicable

If the load surpasses the critical value, $F > F_{\mathrm{cr}}$, the sinus-like beam deflection gets larger and larger, and our equations for small deflection are no longer valid. In fact, the rod will buckle. The straight rod still is a solution to the problem, but it is unstable.

This phenomenon of spontaneous symmetry breaking was discovered by Leonhard Euler. We speak of spontaneous symmetry breaking because the mapping $X \rightarrow -X$ is a symmetry of the differential equation (4.51) as well as of the boundary conditions (4.52). If X is as good as $-X$, we expect the solution $X = 0$. This is true for forces below the critical value. If the force, however, attains the critical value, there are competing non-symmetric solutions. The symmetry is broken spontaneously and not by applying a lateral force K_x. See Fig. 4.1 for this bifurcation type instability.

By the way, if I_x should be smaller than I_y, buckling occurs in the y, z plane, and the critical force is expression (4.54) wit I_x instead of I_y. The critical force depends on the boundary conditions for the rod. For example, if both ends are clamped, one obtains

$$F_{\mathrm{cr}} = \frac{4\pi^2 E I_y}{\ell^2}. \tag{4.56}$$

This appears to be reasonable. A rod which is clamped at both ends should be less prone to buckling.

4.3 Bernoulli's Law

Daniel Bernoulli was a member of a large family of learned persons who lived in various European countries: The Netherlands, Switzerland, Italy, Germany, Russia and others. His most famous book is *Hydrodynamica* which was published in 1738 in Latin and contains the well-known law which is related with his name. It states, in modern language, that the sum of the kinetic energy density and pressure remains constant if the material point travels along its streamline:

$$\frac{\varrho}{2}\boldsymbol{v}^2 + p = \text{const.} \tag{4.57}$$

The assumptions for this to be true are

- The medium is a fluid.
- The fluid is incompressible.
- It is also inviscid, i.e., there is no internal friction or it can be neglected.
- The velocity field is stationary.

An incompressible medium has an invariable mass density, its velocity field must be divergence free:

$$\partial_i v_i = 0. \tag{4.58}$$

Interestingly, we must not resort to this.

The stress tensor $T_{ik} = T'_{ik} + T''_{ik}$ has two contributions. The latter, which describes internal friction, vanishes by assumption. The former is given by

$$T'_{ik} = -p\delta_{ik}, \tag{4.59}$$

where p denotes the pressure field.

With these simplifications the momentum balance equation is

$$\varrho v_i \partial_i v_k = -\partial_k p, \tag{4.60}$$

where we ignore external forces for the moment.

Now, because we consider a stationary situation, the effect of ∂_t vanishes, and the substantial time derivative operator is

$$\mathrm{D}_t = v_i \partial_i . \tag{4.61}$$

Therefore,

$$\varrho\, \mathrm{D}_t\, v_k = -\partial_k p \tag{4.62}$$

holds true and consequently

$$\mathrm{D}_t \, \frac{\varrho}{2} v_k v_k = \varrho v_k \, \mathrm{D}_t \, v_k = -v_k \partial_k p = -\mathrm{D}_t \, p. \tag{4.63}$$

This is Bernoulli's law:

$$\mathrm{D}_t \, \left\{ \frac{\varrho}{2} \boldsymbol{v}^2 + p \right\} = 0. \tag{4.64}$$

The sum of kinetic energy density and pressure for a material point is constant as observed by a co-moving observer. Recall that this has been demonstrated only for an incompressible inviscid fluid and for a stationary velocity field:

- Stationary, because we have set $\partial_t = 0$.
- Inviscid, because we did not take T''_{ik} into account.
- Fluid, because we identified T'_{ik} with $-p\delta_{ik}$.
- Incompressible, because we had to treat ϱ as a constant.

If there is an external conservative force field $f_k = -\partial_k \phi$, such as produced by gravitation, than Eq. (4.64) must be changed to

$$\mathrm{D}_t \, \left\{ \frac{\varrho}{2} \boldsymbol{v}^2 + p + \phi \right\} = 0. \tag{4.65}$$

The Bernoulli law is often applied to compressible media as well. Practically all popular explanations of how an airplane wing produces an upward force refer to it. But bear in mind that this is an oversimplification. Engineers who construct airplanes know better.

4.4 Brownian Motion

In 1905 Albert Einstein published three seminal papers in *Annalen der Physik*. One, *On the Electrodynamics of moving bodies*, revolutionized the concept of space and time. Another one, *On a Heuristic Point of View Concerning the Production and Transformation of Light*, suggested that light is made up of particles which we call photons today. The third important paper[4] showed that the molecular theory of heat predicts stochastic motion of particles suspended in a resting liquid.

Small particles which are suspended in water indeed move in a chaotic way. The Scottish botanist Robert Brown had discovered this in 1827 when observing

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[4] *Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen* a rough translation of which is *On the movement of particles suspended in a resting liquid as required by the molecular-kinetic theory of heat.*

Fig. 4.2 A simulated random walk of a Brownian particle. The starting point $(x, y) = (0, 0)$ is marked by a *filled circle*, the end point after 1,000 observations by a *white circle*

pollen grains, although he was not the first. At first this motion[5] was interpreted as a sign of life, but it soon turned out that powders from ancient rocks showed the same phenomenon. It was Albert Einstein who demonstrated that the small particles did not move on their own, but were pushed by the moving molecules of the environment. He predicted that the displacement grows proportional to the square root of time and calculated an expression for the proportionality constant.

His predictions where later experimentally verified and allowed to determine the value of the Boltzmann constant k_B. Since Avogadro's number N_A, the number of particles for one mole, is related with the universal gas constant[6] by $R = N_\mathrm{A} k_\mathrm{B}$, the mass of the proton could be calculated. Einstein's investigation of Brownian motion was the first concrete step to relate continuum physics with particle physics. For this reason I have included the present article. Diffusion is mass-wise Brownian motion. Brownian motion is diffusion of a single particle. Figure 4.2 shows such a random walk.

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[5] The term *Brownian movement* is used in the literature as well.

[6] A diluted gas of ν moles at temperature T within a vessel of volume V exerts a pressure $p = \nu R T V$.

4.4.1 Einstein's Explanation

So let us reconstruct Einstein's arguments. In order to keep the discussion as simple as possible, we restrict ourselves to the motion in one dimension.

At time $t = 0$ the Brownian particle is at rest and situated at $x = 0$. After a time interval τ_1 it suffers a collision with a molecule of the environment which translates it by s_1, until, after a time interval τ_2, it suffers another collision which translates it by s_2, and so forth.

After the nth collision the Brownian particle has been moved by the environment to

$$x_n = \sum_{j=1}^{n} s_j\,, \tag{4.66}$$

and this location corresponds to time

$$t_n = \sum_{j=1}^{n} \tau_j\,. \tag{4.67}$$

We assume that the τ_j are independent and equally distributed random variables with expectation value $\langle \tau_j \rangle = \tau$. We likewise assume that the displacements s_j are independent and equally distributed random variables with expectation values $\langle s_j \rangle = 0$ and variance $\langle s_j^2 \rangle = s^2$.

The law of large numbers states

$$\lim_{n\to\infty} \frac{t_n}{n} = \tau. \tag{4.68}$$

The central limit theorem states that the probability distribution $p_n(z)$ for $x_n/\sqrt{n}$ converges towards the normal distribution $p(z)$ with variance s^2 which is

$$p(z) = \frac{1}{\sqrt{2\pi s^2}}\, \mathrm{e}^{-z^2/2s^2}\,. \tag{4.69}$$

The probability distribution for the location x_n therefore is

$$G_n(x) \approx \frac{1}{\sqrt{2\pi n s^2}}\, \mathrm{e}^{-x^2/2ns^2}\,. \tag{4.70}$$

We replace n by t/τ, according to Eq. (4.68), and obtain for the limit of G_n the following expression:

$$G(t,x) = \frac{1}{\sqrt{4\pi Dt}}\, \mathrm{e}^{-x^2/4Dt}\,. \tag{4.71}$$

We have set

$$D = \frac{s^2}{2\tau}. \tag{4.72}$$

Recall that $\tau = \langle \tau_j \rangle$ is the average time between collisions of the environment's molecules with the Brownian particle. The displacement of the Brownian particle between two subsequent collision $\langle s_j \rangle$ vanishes on the average. However, its variance $\langle s_j^2 \rangle = s^2$ is positive.

The Brownian particle, which at time $t = 0$ was located at $x = 0$, will be found later within the interval $[x, x + \mathrm{d}x]$ with probability $\mathrm{d}x\, G(t, x)$.

In three dimension Eq. (4.71) reads

$$G(t, \boldsymbol{x}) = G(t, x_1)\, G(t, x_2)\, G(t, x_3) = (4\pi Dt)^{-3/2}\, \mathrm{e}^{-\boldsymbol{x}^2/4Dt}. \tag{4.73}$$

This function obeys the diffusion equation

$$\dot{G} = D\, \Delta G \tag{4.74}$$

with the initial condition

$$G(0, \boldsymbol{x}) = \delta^3(\boldsymbol{x}). \tag{4.75}$$

With $n_0 = n(0, \boldsymbol{x})$ as the initial distribution of particles we easily arrive at the following expression for the particle distribution at time t:

$$n(t, x) = \int \mathrm{d}^3 y\, G(t, \boldsymbol{x} - \boldsymbol{y})\, n_0(\boldsymbol{y}). \tag{4.76}$$

Indeed, Eq. (4.74) warrants that Eq. (4.76) satisfies the diffusion equation, and Eq. (4.75) guarantees $n(0, \boldsymbol{x}) = n_0(\boldsymbol{x})$.

We have plotted in Fig. 4.3 a simulated cloud of identical Brownian particles which all have started at the same point and randomly walked for a certain time in the x, y-plane.

Back to Eq. (4.71). We work out

$$\langle x(t)^2 \rangle = \int dx\, G(t, x)\, x^2 = 2Dt. \tag{4.77}$$

Hence the Brownian particle, as observed in the x, y plane of the microscope, drifts away from its origin according to

$$r(t) = \sqrt{\langle x(t)^2 \rangle + \langle y(t)^2 \rangle} = 2\sqrt{Dt}. \tag{4.78}$$

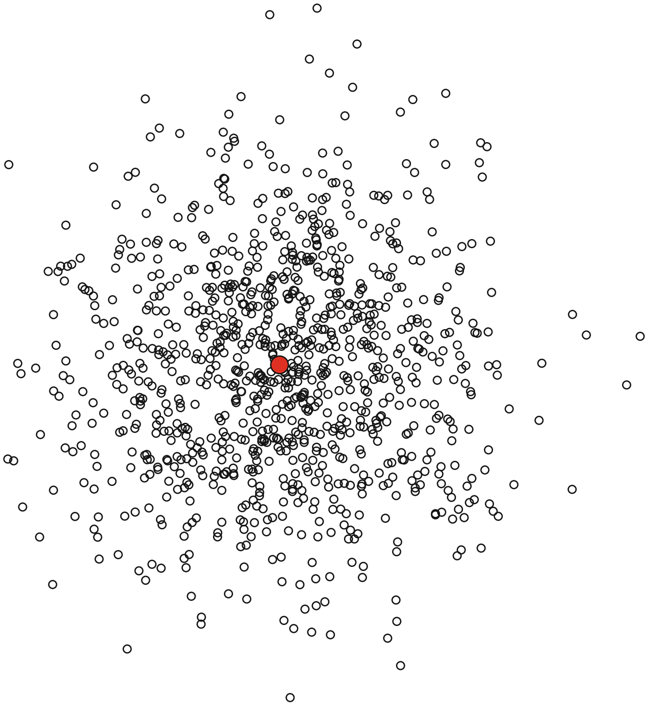

Fig. 4.3 A cloud of 1,000 Brownian particles which all started at the same location (*filled circle*). Their positions in the (x, y)-plane after a certain time are represented by *small white circles*. Diffusion is mass-wise Brownian motion

This formula was Einstein's first contribution to the theory of Brownian motion: the square root time dependence, and not to underestimate, the interpretation in terms of expectation values. A measurement of Brownian motion must be repeated very often such that the averaged results become reliable.

4.4.2 The Diffusion Coefficient

We now recapitulate Einstein's arguments for the interpretation of the diffusion coefficient D.

The Brownian particles are spheres of radius R and effective mass[7] m. They swim in a medium with viscosity η and temperature T.

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[7] True mass minus mass of displaced liquid.

According to the rules of thermodynamics the density of Brownian particles at height z is

$$n(z) = n(0)\,\mathrm{e}^{-mgz/k_\mathrm{B}T}\,. \tag{4.79}$$

This will produce a diffusion current density

$$j^\mathrm{d}(z) = -Dn'(z) = \frac{Dmg}{k_\mathrm{B}T}n(z). \tag{4.80}$$

On the other hand, Brownian particles fall down with a velocity v which is governed by $mg = 6\pi\eta Rv$. See the article on *Stokes' law*. The corresponding sedimentation current density is

$$j^\mathrm{s}(z) = -\frac{mg}{6\pi\eta R}n(z). \tag{4.81}$$

In equilibrium the two currents densities must add up to zero. This is indeed so if

$$D = \frac{k_\mathrm{B}T}{6\pi\eta R} \tag{4.82}$$

holds true.

This result is rather plausible. The higher the temperature, the more the environment will act upon the Brownian particle. If its radius becomes larger, the less it will respond to pushes of its environment. And likewise, the larger the viscosity of the environment, the less the particle moves when pushed.

Since the diffusion constant D, temperature T, viscosity η and the radius R for spherical test particles can be measured, Eq. (4.82) indeed allows to determine the value of the Boltzmann constant k_B and therewith Avogadro's number N_A. Perrin's experiments won him the 1926 physics Nobel prize "for his work on the discontinuous structure of matter, and especially for his discovery of sedimentation equilibrium".

4.4.3 Langevin's Approach

Paul Langevin, a French physicist, has discussed Brownian motion as a stochastic process. The velocity $v = v(t)$ of the Brownian particle is a random variable depending on time. It obeys the following stochastic differential equation:

$$m\dot{v} + \Gamma v = f(t), \tag{4.83}$$

where m is the particle's mass, $\varGamma = 6\pi\eta R$ the friction constant, and $f = f(t)$ is the force exerted by the medium on the particle. It is a stochastic process as well.

Let us digress first on the correlation function of a random process $A = A(t)$. The liquid in which the Brownian particle drifts is in thermal equilibrium, its state is therefore stationary. Expectation values do not depend on time, $\bar{A} = \langle\, A(t)\,\rangle$ is a constant. It is therefore sufficient to discuss the fluctuation $a(t) = A(t) - \bar{A}$ of the random process. The correlation function of such a stationary random process is defined by

$$K_A(\tau) = \langle\, a(t+\tau)\, a(t)\,\rangle. \tag{4.84}$$

Expectation values do *not* depend on time t, but only on the time difference τ.

With

$$a(t) = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t}\, \tilde{a}(\omega) \tag{4.85}$$

we write

$$K_A(\tau) = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{-\mathrm{i}\omega\tau} \int \frac{\mathrm{d}\omega'}{2\pi}\, \mathrm{e}^{\mathrm{i}\omega' t}\, \langle\, \tilde{a}(\omega)\, \tilde{a}^*(\omega')\,\rangle. \tag{4.86}$$

This expression will depend on time t unless

$$\langle\, \tilde{a}(\omega)\, \tilde{a}^*(\omega')\,\rangle = 2\pi\delta(\omega - \omega')\, S_A(\omega) \tag{4.87}$$

holds true. $S_A(\omega)$ is the spectral intensity of the stochastic process under discussion. It is a positive[8] function.

Inserting Eq. (4.87) into Eq. (4.86) yields

$$K_A(\tau) = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega\tau}\, S_A(\omega). \tag{4.88}$$

The correlation function is the Fourier transform of a positive spectral density. This is the Wiener-Khinchin theorem as discussed in Chap. 3.

Let us now return to our discussion of Langevin's approach to Brownian motion. We assume[9]

$$K_f(\tau) = \langle\, f(t+\tau)\, f(t)\,\rangle = \kappa\, \delta(\tau). \tag{4.89}$$

There are two time scales. The interaction of a colliding water molecule with the Brownian particle lasts only an extremely short time, and succeeding collisions

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[8] More accurately: non-negative.

[9] Note that $t \to f(t)$ describes a fluctuation since $\langle\, f(t)\,\rangle = 0$.

are statistically independent. On the other hand, the position of the Brownian particle can be observed only in time intervals of milliseconds, or so. Therefore, from the observers point of view, the correlation function of the force can be well approximated by a δ-function. By the way, the Fourier transform of Eq. (4.89) is κ, a positive constant. Because it does not depend on ω we call $f = f(t)$ a white noise[10] process.

We Fourier transform Langevin's equation (4.83) and obtain

$$(-\mathrm{i}m\omega + \Gamma)\,\tilde{v}(\omega) = \tilde{f}(\omega), \tag{4.90}$$

hence the spectral densities are related by

$$S_v(\omega) = \frac{\kappa}{m^2\omega^2 + \Gamma^2}. \tag{4.91}$$

The Fourier transform of S_v is

$$K_v(\tau) = \frac{\kappa}{m\Gamma}\,\mathrm{e}^{-\Gamma|\tau|/m}. \tag{4.92}$$

As is well known, the translational degree of freedom of a particle is associated with an energy $k_\mathrm{B}T/2$, therefore

$$K_v(0) = \langle\, v(t)^2 \,\rangle = mk_\mathrm{B}T \tag{4.93}$$

holds true, i.e.,

$$K_v(\tau) = \frac{k_\mathrm{B}T}{m}\,\mathrm{e}^{-\Gamma|\tau|/m}. \tag{4.94}$$

Now, we are interested primarily in the displacement of the Brownian particle which is

$$x(t) = \int_0^t \mathrm{d}s\, v(s). \tag{4.95}$$

Clearly, its expectation value $\langle\, x(t) \,\rangle$ vanishes because of $\langle\, v(s) \,\rangle = 0$. So let us calculate[11]

$$\langle\, x(t)^2 \,\rangle = \int_0^t \mathrm{d}s \int_0^t \mathrm{d}s' \,\langle\, v(s)\, v(s') \,\rangle, \tag{4.96}$$

---

[10] The electromagnetic field of white light has a spectral density which, at least in the visible region, does not depend on ω, or color.

[11] We cannot rely on the statement that expectation values do not depend on time. In fact, demanding $x(0) = 0$ breaks time translation symmetry.

the integrand being the velocity correlation function $K_v(s - s')$. Because it is symmetric, we rewrite the right hand side as

$$2\int_0^t \mathrm{d}s \int_0^s \mathrm{d}s'\, K_v(s - s'), \tag{4.97}$$

that is

$$\frac{2k_\mathrm{B}T}{m} \int_0^t \mathrm{d}s\; \mathrm{e}^{-\Gamma s/m} \int_0^s \mathrm{d}s'\; \mathrm{e}^{\Gamma s'/m}\,. \tag{4.98}$$

The result is

$$\langle\, x(t)^2 \,\rangle = \frac{2k_\mathrm{B}T}{\Gamma} \left\{ \frac{m}{\Gamma} - \frac{m}{\Gamma}\,\mathrm{e}^{-\Gamma t/m} + t \right\}. \tag{4.99}$$

Indeed, $\langle\, x(0)^2 \,\rangle = 0$. However, after a short start-up phase, $\langle\, x(t)^2 \,\rangle$ increases linearly with time with a proportionality constant which coincides with Einstein's finding.

Have a look on an interesting paper by Newburgh et al. [8] who have to say more on the subject.

4.5 Bulk and Surface Acoustic Waves in Solids

We show that an isotropic elastic medium allows for longitudinally and transversely polarized sound waves and discuss their attenuation. The wave equation also has solutions which are concentrated beneath a surface.

4.5.1 Wave Equation

Recall the momentum balance equation (1.75), namely

$$\varrho\, \mathrm{D}_t\, v_i = \partial_j T_{ij} + f_j\,, \tag{4.100}$$

where ϱ is the mass density, v_i the flow velocity, $T_{ij} = T_{ji}$ the stress tensor and f_i an external force per unit volume. D_t denotes the substantial time derivative. Hence $\mathrm{D}_t\, v_i$ is the acceleration as observed by a co-moving observer.

We specialize to an isotropic elastic medium. f_i will play no role. Since the displacement u_i of material points is and remains small, we may write $\mathrm{D}_t\, v_i = \ddot{u}_i$, so that we have to solve

$$\varrho \ddot{u}_i = \partial_j T_{ij}\,. \tag{4.101}$$

For the beginning, let us neglect the irreversible contribution to the stress tensor, i.e., internal friction. An isotropic medium then is described by

$$T_{ij} = \frac{E}{1+\nu}\left\{S_{ij} + \frac{\nu}{1-2\nu}\delta_{ij}S_{kk}\right\}, \tag{4.102}$$

with

$$S_{ij} = \frac{\partial_i u_j + \partial_j u_i}{2}. \tag{4.103}$$

Inserting Eq. (4.103) into Eq. (4.102) and this into Eq. (4.101) results in

$$\varrho \ddot{u}_i = \frac{E}{2(1+\nu)}\Delta u_i + \frac{\nu E}{(1+\nu)(1-2\nu)}\partial_i \partial_j u_j\,. \tag{4.104}$$

$\Delta = \partial_j \partial_j$ is the Laplacian. We introduce the Lamé parameters[12]

$$\mu = \frac{E}{2(1+\nu)} \tag{4.105}$$

and

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}. \tag{4.106}$$

With it Eq. (4.104) reads

$$\varrho \ddot{u}_i = \mu \Delta u_i + (\lambda + \mu)\partial_i \partial_k u_k\,. \tag{4.107}$$

This is a linear wave equation.

4.5.2 Bulk Acoustic Waves

Any field can be decomposed into plane waves:

$$\boldsymbol{u}(t,\boldsymbol{x}) = \boldsymbol{a}\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}\,. \tag{4.108}$$

A linear wave equation gives rise to a relation between angular frequency and wave vector, $\omega = \omega(\boldsymbol{q})$. In our case the wave equation reads

$$\varrho \omega^2 a_i = \mu q^2 a_i + (\lambda + \mu) a_k q_k q_i\,. \tag{4.109}$$

There are two eigensolutions.

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[12] Note that μ coincides with the shear modulus which is also denoted by G. While elasticity moduli are isothermal quantities, the Lamé parameters refer to adiabatic thermodynamic processes.

If we choose $\boldsymbol{a} \parallel \boldsymbol{q}$, we arrive at a mode with

$$\omega = c_{\parallel} q \text{ where } c_{\parallel} = \sqrt{\frac{\lambda + 2\mu}{\varrho}}. \tag{4.110}$$

The solution for $\boldsymbol{a} \perp \boldsymbol{q}$ is given by

$$\omega = c_{\perp} q \text{ where } c_{\perp} = \sqrt{\frac{\mu}{\varrho}}. \tag{4.111}$$

Equation (4.110) is the dispersion relation for a longitudinally polarized acoustic wave while Eq. (4.111) refers to a transversal wave. Note that both Lamé constants λ and μ are positive. Therefore, the longitudinally polarized mode travels faster, $c_{\parallel} > c_{\perp}$. In seismology, the longitudinal mode is also called primary while the transversal wave is called secondary. If there is an earthquake, longitudinally polarized and transversal acoustic waves are excited simultaneously. The former, however, will arrive first at a seismic monitoring station because it travels faster.

For aluminum, at 20 °C, longitudinally polarized sound propagates with $c_{\parallel} = 6,374 \text{ m s}^{-1}$, transversely polarized with $c_{\perp} = 3,111 \text{ m s}^{-1}$. These values are taken from the tables of Kaye and Laby [5], published in the Internet by the UK National Physics Laboratory.

4.5.3 *Attenuation*

Let us now briefly discuss an inelastic contribution T''_{ij} to the stress tensor. It must be proportional to the velocity $\dot{u}_i$. The most general form for an isotropic medium is

$$T''_{ij} = \eta_1 \dot{S}_{ij} + \eta_2 \delta_{ij} \dot{S}_{kk}. \tag{4.112}$$

Equation (4.107) will now contain additional terms of $\dot{u}_k$ which show up in Eq. (4.109) as contributions proportional to $-\mathrm{i}\omega$. Again, the modes are polarized either longitudinally or transversely. However, for real ω, there is no longer a real solution for $\boldsymbol{q}$. Instead, $q = k + \mathrm{i}\alpha/2$ acquires a small imaginary part such that the plane wave becomes

$$u_i(t, \boldsymbol{x}) \propto \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{\mathrm{i}k\boldsymbol{n}\cdot\boldsymbol{x}}\, \mathrm{e}^{-\alpha\boldsymbol{n}\cdot\boldsymbol{x}/2}. \tag{4.113}$$

$\boldsymbol{n}$, a unit vector, describes the propagation direction. Since the power carried by the acoustic wave is proportional to $|\boldsymbol{u}|^2$, this will decrease exponentially with the propagation length, the decay coefficient being α. Kaye and Laby [5] cite $\alpha = 0.40 \text{ m}^{-1}$ for aluminum at 40 MHz.

4.5.4 Rayleigh Waves

Assume an isotropic elastic medium in the half space $x > 0$, and vacuum below. The surface $x = 0$ can guide acoustic waves the amplitudes of which decrease rapidly with $x \to \infty$ and may travel freely in the y, z-plane. Without loss of generality we choose z to be the direction of propagation.[13] Here we shall study in detail so-called Rayleigh surface acoustic waves. We will also comment on generalizations and applications.

One must look for a solution of the wave equation (4.107). Any linear combination of longitudinally and transversely polarized waves will do. We require that the wave number $q_3 = k$ is the same for both types. Hence the wave vectors are

$$\boldsymbol{q}_{\parallel} = \begin{pmatrix} \mathrm{i}\kappa_{\parallel} \\ 0 \\ k \end{pmatrix} \text{ and } \boldsymbol{q}_{\perp} = \begin{pmatrix} \mathrm{i}\kappa_{\perp} \\ 0 \\ k \end{pmatrix}, \tag{4.114}$$

where

$$\omega^2 = c_{\parallel}^2 (k^2 - \kappa_{\parallel}^2) = c_{\perp} (k^2 - \kappa_{\perp}^2). \tag{4.115}$$

Both expressions, namely

$$\boldsymbol{u}_{\parallel}(t, \boldsymbol{x}) = \begin{pmatrix} -\kappa_{\parallel} \\ 0 \\ \mathrm{i}k \end{pmatrix} \mathrm{e}^{-\kappa_{\parallel} x} \, \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{e}^{\mathrm{i}kz} \tag{4.116}$$

and

$$\boldsymbol{u}_{\perp}(t, \boldsymbol{x}) = \begin{pmatrix} \mathrm{i}k \\ 0 \\ \kappa_{\perp} \end{pmatrix} \mathrm{e}^{-\kappa_{\perp} x} \, \mathrm{e}^{-\mathrm{i}\omega t} \, \mathrm{e}^{\mathrm{i}kz}, \tag{4.117}$$

satisfy the wave equation. In Eq. (4.117) we have chosen a vector with vanishing y-component, which defines a Rayleigh surface acoustic wave, namely

$$\boldsymbol{u}(t, \boldsymbol{x}) = A_{\parallel} \boldsymbol{u}_{\parallel}(t, \boldsymbol{x}) + A_{\perp} \boldsymbol{u}_{\perp}(t, \boldsymbol{x}). \tag{4.118}$$

However, there are boundary conditions to be taken into account. The momentum flux through the surface $x = 0$ must vanish, which means $T_{11} = T_{21} = T_{31} = 0$ at $x = 0$. Put otherwise, there are no forces acting from outside on the surface.

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[13] We freely mix $\boldsymbol{x} = (x_1, x_2, x_3) = (x, y, z)$.

Now, T_{21} vanishes entirely in our situation. $T_{31} = 0$ at $x = 0$ means

$$\partial_1 u_3 + \partial_3 u_1 = 0 \text{ for } x = 0, \tag{4.119}$$

or

$$2\mathrm{i}k\kappa_{\|} A_{\|} + (k^2 + \kappa_{\perp}^2) A_{\perp} = 0. \tag{4.120}$$

The remaining boundary condition $T_{11} = 0$ at $x = 0$ reads

$$2\mu\, \partial_1 u_1 + \lambda(\partial_1 u_1 + \partial_3 u_3) = 0. \tag{4.121}$$

With $\varrho c_{\|}^2 = \lambda + 2\mu$ and $\varrho c_{\perp}^2 = \mu$ we rewrite this as

$$c_{\|}^2\, \partial_1 u_1 + (c_{\|}^2 - 2c_{\perp}^2)\, \partial_3 u_3 = 0. \tag{4.122}$$

Resorting to Eq. (4.118) we calculate

$$((c_{\|}^2 - 2c_{\perp}^2)k^2 - c_{\|}^2\kappa_{\|}^2)A_{\|} + 2c_{\perp}^2 \mathrm{i}k\kappa_{\perp} A_{\perp} = 0. \tag{4.123}$$

The factor in front of $A_{\|}$ may be reformed into $-c_{\perp}^2(k^2 + \kappa_{\perp}^2)$ so that Eq. (4.123) becomes

$$(k^2 + \kappa_{\perp}^2)A_{\|} - 2\mathrm{i}k\kappa_{\perp} A_{\perp} = 0. \tag{4.124}$$

The boundary conditions (4.120) and (4.124) have a non-trivial solution if and only if the determinant of the coefficient matrix vanishes:

$$\det \begin{pmatrix} 2\mathrm{i}k\kappa_{\|} & k^2 + \kappa_{\perp}^2 \\ k^2 + \kappa_{\perp}^2 & -2\mathrm{i}k\kappa_{\perp} \end{pmatrix} = 4k^2\kappa_{\|}\kappa_{\perp} - (k^2 + \kappa_{\perp}^2)^2 = 0. \tag{4.125}$$

Let us express this in terms of sound speed $v = \omega/k$:

$$\sqrt{1 - \frac{v^2}{c_{\|}^2}}\sqrt{1 - \frac{v^2}{c_{\perp}^2}} = \left(1 - \frac{v^2}{2c_{\perp}^2}\right)^2. \tag{4.126}$$

v must be smaller than $c_{\perp}$ in order to guarantee real values for $\kappa_{\|}$ and $\kappa_{\perp}$. Figure 4.4 depicts the left hand and right hand side of Eq. (4.126).

There is exactly one solution to Eq. (4.126), namely $v = c_{\mathrm{R}} = 2{,}906\ \mathrm{m\,s^{-2}}$ for aluminum. The speed of sound of the Rayleigh surface acoustic wave for aluminum coincides with the value cited by Kaye and Laby [5] which, I hope, was measured and not calculated.

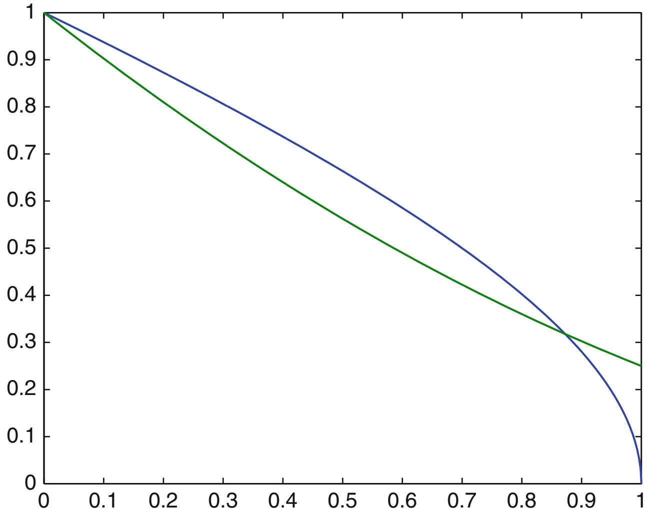

Fig. 4.4 The *left* and *right hand sides* of Eq. (4.126) are plotted over $v^2/c_\perp^2$ for aluminum. The intersection defines the speed of the Rayleigh surface acoustic wave

4.5.5 More on SAW

Surface acoustic waves, or SAW, is a topic for research and application in various branches of science. Here we can only touch some of them.

Even for isotropic media, there are two types of surface acoustic wave, Rayleigh and Love waves. The former have been dealt with in detail. The latter is described by

$$\boldsymbol{u}_\perp(t,\boldsymbol{x}) = \begin{pmatrix}0\\k\\0\end{pmatrix} \mathrm{e}^{-\kappa_\perp x}\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}kz} \tag{4.127}$$

instead of Eq. (4.117). We will not run through the above procedure again.

In the field of seismology, acoustic surface waves are among the main topics. If an earthquake happens somewhere, then bulk elastic waves and surface waves are excited. The longitudinally polarized elastic wave is the fastest, its transversely polarized counterpart is slower. Bulk elastic waves spread out in space, their intensity falls off like $1/r^2$ with distance r. Surface waves are even slower. However, they spread out on a surface, thus their intensity decreases as $1/r$ only. Moderately far away from the epicenter of an earthquake, surface waves carry more energy than bulk waves. The surface waves cause destruction, but they are announced by bulk waves.

Surface acoustic waves are also of interest in electronics, in particular, if stress is accompanied by electric phenomena.

Electric effects, such as piezoelectricity, are described by a relation

$$E_i = P_{ijk} T_{jk}, \tag{4.128}$$

a linear relationship between the electric field strength E_i and the stress tensor T_{jk}. Only crystals which lack inversion symmetry allow for a tensor P_{ijk} of rank three. Among them are quartz and lithium niobate. Equation (4.128) allows for the excitation of surface acoustic waves by electric fields and for their electric detection. Filters, oscillators, transformers and transducers are commercial applications. Each mobile phone contains an SAW based oscillator. Scientifically, the identification of surface acoustic waves for non-isotropic crystals is still not yet complete.

4.6 Crystal Optics

The optical properties of a transparent continuum are described by its susceptibility tensor χ_{ij}. We have shown in Chap. 3 how to calculate it from first principles within the framework of quantum mechanics and statistical thermodynamics. Although it is impossible to work out the relevant expectation values exactly, a number of features are true in general. We summarize them and present consequences for the propagation of light.

4.6.1 Susceptibility

The electric polarization field $P_i = P_i(t, \boldsymbol{x})$ depends, in first order perturbation theory, linearly on the electric field $E_i = E_i(t, \boldsymbol{x})$ of a light wave:

$$P_j(t, \boldsymbol{x}) = \int_0^\infty \mathrm{d}\tau \int \mathrm{d}^3\boldsymbol{\xi} \sum_k \Gamma_{jk}(\tau, \boldsymbol{\xi})\, E_k(t - \tau, \boldsymbol{x} - \boldsymbol{\xi}). \tag{4.129}$$

Note that the polarization depends on previous perturbations only (causal solution). By Fourier transforming Eq. (4.129) we obtain

$$\tilde{P}_j(\omega, \boldsymbol{q}) = \epsilon_0 \sum_k \chi_{jk} \tilde{E}(\omega, \boldsymbol{q}), \tag{4.130}$$

where $\chi_{jk} = \chi_{jk}(\omega, \boldsymbol{q})$ is the susceptibility tensor of the medium under investigation. ω and $\boldsymbol{q}$ are angular and spatial frequencies.

We shall decompose the susceptibility tensor into its Hermitian and anti-Hermitian parts,

$$\chi_{jk} = \chi'_{jk} + \mathrm{i}\, \chi''_{jk}. \tag{4.131}$$

χ'_{jk} is called the refractive part because it causes refraction of light. The dissipative or absorptive part χ''_{jk} causes absorption. Both parts are Hermitian tensors, they obey $H_{ij} = H^*_{ji}$.

The refractive part is intimately related with the absorptive part by the dispersion, or Kramers-Kronig relation:

$$\chi'_{jk}(\omega, \boldsymbol{q}) = \mathrm{Pr} \int_0^\infty \frac{\mathrm{d}u}{\pi} \frac{2u\, \chi''_{jk}(u, \boldsymbol{q})}{u^2 - \omega^2}. \tag{4.132}$$

Pr denotes the principal value integral.

As mentioned earlier, the susceptibility is an expectation value with respect to the system's equilibrium, or Gibbs state. It therefore depends on all parameters which determine the Gibbs state, such as temperature T, strain S_{ij}, external electric field and magnetic induction $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{B}}$, respectively, and so forth. Onsager's reciprocity theorem states

$$\chi_{jk}(\omega, \boldsymbol{q}; \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}) = \chi_{kj}(\omega, \boldsymbol{q}; \boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}). \tag{4.133}$$

The susceptibility tensor is symmetric under exchange of its indexes, provided an external quasi-static magnetic induction is reversed as well.

We will discuss in the following the case $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{B}} = \boldsymbol{q} = 0$. Effects which are linear in $\boldsymbol{\mathcal{E}}$ are dealt with in an article on the *Pockels effect*. Another article on the *Faraday effect* discusses a linear dependency of the susceptibility on a quasi-static magnetic induction $\boldsymbol{\mathcal{B}}$. And finally, a first order addition proportional to $\boldsymbol{q}$ is the subject of an article on *Optical activity*.

4.6.2 Planar Waves

The permittivity tensor $\epsilon_{jk}(\omega) = \delta_{jk} + \chi_{jk}(\omega)$ appears in Maxwell's equations. Each component $F = F(t, \boldsymbol{x})$ of the electromagnetic field may be decomposed into contributions with definite angular frequency ω and spatial frequencies $\boldsymbol{k} = (k_1, k_2, k_3)$,

$$F(t, \boldsymbol{x}) = \int \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{d}^3 k}{(2\pi)^3} f(\omega, \boldsymbol{k})\, \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}. \tag{4.134}$$

In particular, the electric field strength $\boldsymbol{e} = \boldsymbol{e}(\omega, \boldsymbol{k})$ has to obey

$$\{\boldsymbol{k} \times \boldsymbol{k} \times \boldsymbol{e}\}_j = \frac{\omega^2}{c^2} \epsilon_{jk} e_k. \tag{4.135}$$

Here $c = 1/\sqrt{\epsilon_0 \mu_0}$ is the vacuum speed of light. Equation (4.135) is a dispersion, or mode equation. For given ω only certain spatial frequencies $\boldsymbol{k}$ are allowed. The direction $\hat{\boldsymbol{e}}$ of $\boldsymbol{e}$, a unit vector, describes the polarization of the plane wave. Note that $\hat{\boldsymbol{e}}$ and $-\hat{\boldsymbol{e}}$ describe the same polarization. This is reflected by Eq. (4.135) which should be rewritten in terms of the polarization vector $\hat{\boldsymbol{e}}$ instead of the electric field strength[14] $\boldsymbol{e}$.

ω/c is usually abbreviated by k_0. It is called the vacuum wave number because of $\omega/c = |\boldsymbol{k}|$ for the propagation of electromagnetic waves in vacuum. Let us write $\boldsymbol{k} = nk_0\hat{\boldsymbol{k}}$ with n the refractive index and $\hat{\boldsymbol{k}}$ the propagation direction. With this abbreviations, Eq. (4.135) reads now

$$n^2\{\hat{\boldsymbol{k}} \times \hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}\}_j = \epsilon_{jk}\hat{e}_k. \tag{4.136}$$

4.6.3 Optical Isotropy

A transparent, optically inactive medium is described by a real symmetric permittivity tensor ϵ_{jk}. This holds true if no quasi-static external electric or magnetic fields are applied and if the medium suffers no stress.

The permittivity tensor can then be orthogonally diagonalized. There is a Cartesian coordinate systems such that the permittivity tensor is diagonal. There are three cases: all diagonal elements are equal, only two are equal, or all three eigenvalues differ from each other. In the former case one speaks of *optical isotropy*, otherwise of *birefringence*. Here we discuss optically isotropic media.

The permittivity has the form

$$\epsilon_{jk}(\omega) = \epsilon(\omega)\delta_{jk}, \tag{4.137}$$

with respect to *any* Cartesian system of reference.

The mode equation (4.136) now reads

$$n^2\{\hat{\boldsymbol{k}} \times \hat{\boldsymbol{k}} \times \hat{\boldsymbol{e}}\} = \epsilon\,\hat{\boldsymbol{e}}. \tag{4.138}$$

Recall that $\boldsymbol{k} = nk_0\hat{\boldsymbol{k}}$ is the wave vector of the plane wave, $\omega = k_0 c$ the corresponding angular frequency, and $\hat{\boldsymbol{e}}$ denotes the polarization vector.

Equation (4.138) demands that $\hat{\boldsymbol{k}}$ and $\hat{\boldsymbol{e}}$ are orthogonal,

$$\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{e}} = 0, \tag{4.139}$$

as well as

$$n = \sqrt{\epsilon}. \tag{4.140}$$

Light propagating in an isotropic medium is transversely polarized. Any propagation direction $\hat{\boldsymbol{k}}$ is admissible. The wave number $|\boldsymbol{k}|$ is larger than that in vacuum by a factor $n = \sqrt{\epsilon}$. The refractive index $n = n(\omega)$ of the plane wave solution in

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[14] More precisely, its Fourier transform.

general depends on the angular frequency ω. This gives rise to the phenomenon of dispersion in a beam made up of light of different colors, such as sun light.

Ordinary glass is transparent within the spectral range of visible light and optically isotropic. Its permittivity depends on ω and on composition. A refractive index $n = 1.50$ is a typical value.

4.6.4 *Birefringence*

Amorphous substances and cubic crystals, such as NaCl (ordinary salt), are optically isotropic. Crystals with a more complex symmetry, such as lithium niobate, exhibit two different eigenvalues of the permittivity tensor. Even more complex crystals, such as potassium niobate, may have three distinct eigenvalues.

Here we discuss in more detail the case of two equal eigenvalues ϵ_o which differ from the third ϵ_e. There is a Cartesian coordinate system such that the permittivity tensor is described by

$$\epsilon_{jk} = \begin{pmatrix} \epsilon_\mathrm{o} & 0 & 0 \\ 0 & \epsilon_\mathrm{o} & 0 \\ 0 & 0 & \epsilon_\mathrm{e} \end{pmatrix}. \tag{4.141}$$

We have to solve the dispersion equation (4.136). Note that there is a preferred axis, the so-called optical axis $\hat{\boldsymbol{c}} = (0, 0, 1)$. This is the 3-axis in our notation.

An ordinary beam is described by $\hat{\boldsymbol{k}} = \hat{\boldsymbol{c}}$. Equation (4.138) is satisfied if the polarization vector $\hat{\boldsymbol{e}}$ is perpendicular to the optical axis, i.e., in the 1-2 plane. The ordinary beam propagates with a refractive index

$$n_\mathrm{o} = \sqrt{\epsilon_\mathrm{o}}. \tag{4.142}$$

The ordinary beam travels along the optical axis $\hat{\boldsymbol{c}}$, its polarization is transverse, i.e., perpendicular to the propagation direction. This behavior is considered to be ordinary since, for a given direction of propagation, the polarization may be chosen orthogonal to it, but without further restrictions.

An extraordinary beam is described by $\hat{\boldsymbol{e}} = \hat{\boldsymbol{c}}$. The polarization of the extraordinary beam is along the optical axis. Equation (4.138) again demands that polarization $\hat{\boldsymbol{e}}$ and direction $\hat{\boldsymbol{k}}$ of propagation are orthogonal. Hence, the beam propagates at an arbitrary angle in the 1-2-plane. This behavior, namely fixed polarization and arbitrary propagation perpendicular to it, is considered to be extraordinary. The refractive index for an extraordinary beam is $n_\mathrm{e} = \sqrt{\epsilon_\mathrm{e}}$.

If a light beam passes through the surface of a birefringent material it splits into an ordinary and an extraordinary beam. They travel in possibly different directions with different refractive indexes. A birefringent crystal exhibits double refraction, hence its name. There is one optical axis, because two eigenvalues of the permittivity are equal and differ from the third. Crystals of such a behavior are optically uniaxial.

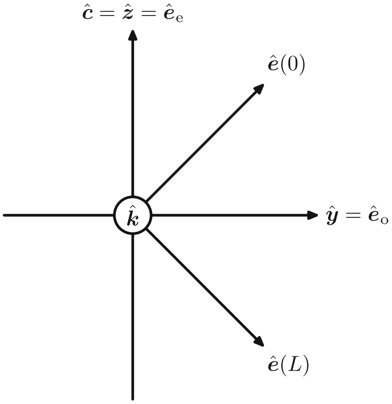

Fig. 4.5 A plane wave propagates along $\hat{\boldsymbol{k}}$ in a birefringent medium with optical axis $\hat{\boldsymbol{c}}$. Initially, the wave is neither ordinary ($\hat{\boldsymbol{e}}_o$) nor extraordinary ($\hat{\boldsymbol{e}}_e$), but a superposition thereof with equal weights. Having propagated a certain length L, the polarization has become orthogonal to the initial direction

There are crystals where all three eigenvalues of the permittivity tensor are different. They have two optical axes and are called optically biaxial. We will not discuss this situation here.

4.6.5 Polarization Change Due to Birefringence

Assume a situation where the wave propagates in 1-direction, $\hat{\boldsymbol{k}} = (1, 0, 0)$ through a medium the optical axis of which is $\hat{\boldsymbol{c}} = (0, 0, 1)$, the 3-axis. At $x = 0$ the plane wave shall be neither ordinary ($\hat{\boldsymbol{e}}_2$) nor extraordinary ($\hat{\boldsymbol{e}}_3$), but a superposition $\hat{\boldsymbol{e}} = \cos\alpha\hat{\boldsymbol{e}}_2 + \sin\alpha\hat{\boldsymbol{e}}_3$. See Fig. 4.5 for a sketch.

The ordinary wave propagates with refractive index n_0, the ordinary with n_e along $\hat{\boldsymbol{k}}$. Therefore,

$$\hat{\boldsymbol{e}}(x) = \mathrm{e}^{-\mathrm{i}nk_0x} \begin{pmatrix} 0 \\ \cos\alpha\,\mathrm{e}^{\mathrm{i}\Delta nk_0x/2} \\ \sin\alpha\,\mathrm{e}^{-\mathrm{i}\Delta nk_0x/2} \end{pmatrix}, \tag{4.143}$$

where $n = (n_o + n_e)/2$ and $\Delta n = (n_o - n_e)$.

Define L by $\Delta nk_0L = \pi/4$. Having propagated this length, the polarization is now

$$\hat{\boldsymbol{e}}(L) = \cos\alpha\hat{\boldsymbol{e}}_2 - \sin\alpha\hat{\boldsymbol{e}}_3. \tag{4.144}$$

In particular, if the angle α is 45°, $\hat{\boldsymbol{e}}(0) = (0, 1, 1)/\sqrt{2}$ has changed into $\hat{\boldsymbol{e}}(L) = (0, 1, -1)/\sqrt{2}$. The polarization at $x = 0$ and at $y = L$ are orthogonal. This effect is exploited in Pockels and Kerr cells where the birefringence parameter Δn can be controlled by an external electric field.

4.6.6 Absorption

Assume that the permittivity[15] has a small imaginary part,

$$\epsilon(\omega) = \epsilon'(\omega) + \mathrm{i}\,\epsilon''(\omega). \tag{4.145}$$

From Eq. (4.138) it follows again that the direction of propagation and the polarization vector are perpendicular, $\hat{\boldsymbol{k}} \perp \hat{\boldsymbol{e}} = 0$. Light in bulk material[16] is transversely polarized.

With $\boldsymbol{k} = \bar{n} k_0 \hat{\boldsymbol{k}}$ as before we conclude $\bar{n}^2 = \epsilon' + \mathrm{i}\,\epsilon''$, or

$$\bar{n} \approx \sqrt{\epsilon'} + \frac{\mathrm{i}\,\epsilon''}{2\sqrt{\epsilon'}}. \tag{4.146}$$

We have made use of $|\epsilon''| \ll |\epsilon'|$. With $z = \hat{\boldsymbol{k}} \cdot \boldsymbol{x}$ as propagation distance we may write our solution as

$$\boldsymbol{E}(t, \boldsymbol{x}) \propto \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{-\alpha z/2}\, \mathrm{e}^{\mathrm{i} k_0 n z}, \tag{4.147}$$

where $n = \sqrt{\epsilon'}$ is the (real) refractive index of the wave and

$$\alpha = \frac{\epsilon''}{n} k_0 \tag{4.148}$$

its absorption, or attenuation constant. Both the refractive index and the absorption constant will depend on frequency.

Since the intensity S of a light beam is proportional to $|\boldsymbol{E}|^2$, it decreases as

$$S(z) = S(0)\, \mathrm{e}^{-\alpha z} \tag{4.149}$$

with propagation distance z.

In the above discussion we always had a dielectric medium in mind. The propagation of light in metals or semi-conductors is another story.

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[15] For simplicity, we assume an optically isotropic medium.

[16] As contrasted with waveguides.

4.6.7 Dispersion

The Kramers-Kronig relation

$$\epsilon'(\omega) = 1 + \operatorname{Pr} \int_0^\infty \frac{\mathrm{d}u}{\pi} \frac{2u\,\epsilon''(u)}{u^2 - \omega^2} \tag{4.150}$$

relates[17] the refractive part ϵ' of the permittivity with the absorptive part ϵ''. Recall that Eq. (4.150) is a consequence of the causality principle.

The absorption of light quanta by matter may be traced back to different effects, such as electronic and vibrational excitations, plasma vibrations, absorption by dye molecules, and so forth. These absorption processes are restricted to broad or narrow frequency ranges, so called bands. By representing such a band r by a central frequency ω_r and a strength f_r, the following representation of Eq. (4.150) is plausible:

$$n(\omega) = 1 + \sum_r f_r \frac{\omega_r^2}{\omega_r^2 - \omega^2}, \tag{4.151}$$

a so called Sellmeier equation. The f_r must be positive numbers because of $\epsilon''(\omega) \geq 0$.

A spectrometer sorts a beam of incident light according to frequency, or wavelength, or color. A simple prism may do this, it relies on $n = n(\omega)$, i.e., on dispersion.

4.7 Dielectric Planar Waveguides

A planar waveguide is characterized by a permittivity profile $\epsilon = \epsilon(x)$ which does not depend on y or z. The wave vector lies in the (y, z) plane, and we choose the z direction without loss of generality. See Fig. 4.6 for an example. All components of the electromagnetic field are shaped according to

$$F(t, x, y, z) = F(x)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}\beta z}. \tag{4.152}$$

Maxwell's equations for vanishing charges and currents and for a non-magnetic medium read

$$\nabla \times \boldsymbol{H} = -\mathrm{i}\omega\epsilon_0\epsilon\,\boldsymbol{E} \text{ and } \nabla \times \boldsymbol{E} = \mathrm{i}\omega\mu_0\,\boldsymbol{E}, \tag{4.153}$$

in usual notation. $\epsilon = \epsilon(x)$ is the relative permittivity. Note that both divergence equations are automatically satisfied if $\omega \neq 0$.

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[17] The principal value symbol Pr specifies how to cope with the singularity at $u = \omega$.

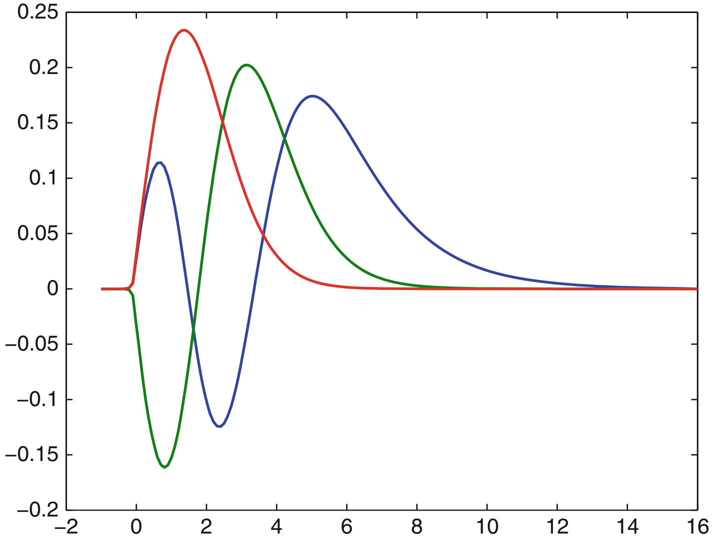

Fig. 4.6 Electric field strength of guided modes vs. depth below surface (microns) of a graded index waveguides. See the `MATLAB` program for waveguide parameters

Just as a free photon has two states of polarization, there are two differently polarized modes, TE and TM. It is the Electric or Magnetic field strength, respectively, which is Transversal, i.e., orthogonal to the waveguide normal as well as to the propagation direction.

A TE mode is specified by

$$\boldsymbol{E} = \begin{pmatrix} 0 \\ E \\ 0 \end{pmatrix} \text{ and } \boldsymbol{H} = \frac{-1}{\omega\mu_0} \begin{pmatrix} \beta E \\ 0 \\ \mathrm{i}\,E' \end{pmatrix}, \tag{4.154}$$

a TM mode by

$$\boldsymbol{H} = \begin{pmatrix} 0 \\ H \\ 0 \end{pmatrix} \text{ and } \epsilon\,\boldsymbol{E} = \frac{1}{\omega\epsilon_0} \begin{pmatrix} \beta H \\ 0 \\ \mathrm{i}\,H' \end{pmatrix}. \tag{4.155}$$

For our geometry, $\epsilon\, E_x$ must be continuous as well as E_y, E_z, H_x, H_y, and H_z. In the case of a TE mode, E and E' must be smooth functions. For a TM mode, H and H'/ϵ have to be continuous.

Recall that all fields here are Fourier components of a decomposition into periodic contributions. Since the space-time dependent fields are real, the components obey $F(\omega) = F^*(-\omega)$. Decomposing the Poynting vector, the energy current density, yields four contributions, varying with 2ω, -2ω, and zero frequency. The latter is

$$\boldsymbol{S} = 2\,\mathrm{Re}\,\boldsymbol{E} \times \boldsymbol{H}^*. \tag{4.156}$$

We will study two different kinds of planar waveguides. A graded index waveguide is characterized by a smoothly varying permittivity profile while a slab waveguides consists of one ore more homogeneous films of different optical properties.

4.7.1 TE Modes

For a TE mode, the electric field strength $E = E(x)$ has to obey

$$\frac{1}{k_0^2} E'' + \epsilon(x) E = \epsilon_{\mathrm{eff}} E. \tag{4.157}$$

This is an eigenvalue problem, the eigenvalue being the effective permittivity $\epsilon_{\mathrm{eff}} = (\beta/k_0)^2$. For a given light source frequency ω, the mode equation (4.157) allows to calculate the possible propagation constants β.

According to Eq. (4.156) the energy current density is

$$S = \frac{2\beta}{\omega\mu_0} |E(x)|^2. \tag{4.158}$$

By integrating over x we obtain the power flux per lateral unit length:

$$\frac{\mathrm{d}P}{\mathrm{d}y} = \frac{2\beta}{\omega\mu_0} \int \mathrm{d}x\; |E(x)|^2. \tag{4.159}$$

It is therefore natural to define the following scalar product:

$$(g, f) = \int \mathrm{d}x\; g^*(x)\, f(x). \tag{4.160}$$

Note that the TE mode operator[18]

$$L_{\mathrm{TE}} = \frac{1}{k_0^2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \epsilon(x) \tag{4.161}$$

is self-adjoint with respect to the scalar product Eq. (4.160). Hence, the ϵ_{eff} are real. Since the second derivative operator is negative,[19] the eigenvalues ϵ_{eff} are smaller

---

[18] L_{TE} is dimensionless which is desirable for numerical investigation.

[19] A is negative if $(f, Af) \le 0$ for all f, here: $(f, f'') = -(f', f') \le 0$.

than the largest permittivity. A guided mode is characterized by $(E, E) < \infty$, by a finite total power flux per unit lateral length. Therefore, ϵ_{eff} must be larger than the permittivities at infinity. Otherwise the solutions would be of sine type at infinity and could not be normalized. The guided mode fields are mutually orthogonal with respect to the scalar product (4.160).

All continuity requirements are fulfilled if $x \to E(x)$ and $x \to E'(x)$ are continuous functions.

4.7.2 TM Modes

For a TM mode, the magnetic field strength has to obey the following mode equation[20]

$$\frac{1}{k_0^2}\,\epsilon\frac{\mathrm{d}}{\mathrm{d}x}\epsilon^{-1}\frac{\mathrm{d}}{\mathrm{d}x}H + \epsilon H = \epsilon_{\text{eff}}H. \tag{4.162}$$

This defines again an eigenvalue problem, the eigenvalue being ϵ_{eff}.

Equation (4.155) implies the following expression for the power flux per lateral unit length:

$$\frac{\mathrm{d}P}{\mathrm{d}y} = \frac{2\beta}{\omega\epsilon_0}\int \mathrm{d}x\;\frac{1}{\epsilon(x)}\,|H(x)|^2. \tag{4.163}$$

It is therefore natural to define the scalar product

$$(g, f) = \int \mathrm{d}x\;\frac{1}{\epsilon(x)}\,g^*(x)\,f(x). \tag{4.164}$$

It is not difficult to show that the TM mode operator

$$L_{\text{TM}} = \frac{1}{k_0^2}\,\epsilon\frac{\mathrm{d}}{\mathrm{d}x}\epsilon^{-1}\frac{\mathrm{d}}{\mathrm{d}x} + \epsilon \tag{4.165}$$

is self-adjoint with respect to the scalar product Eq. (4.164), hence its eigenvalues are real and the eigenvectors are orthogonal with respect to that scalar product.

Again, as for TE modes, the differential operator part of Eq. (4.165) is negative, since $(f, f'') = -(f', f')$ holds true. Therefore, the allowed effective permittivities are smaller than the maximum permittivity and larger than the permittivity at infinity.

All continuity requirements are fulfilled if $x \to H(x)$ and $x \to H'(x)/\epsilon(x)$ are continuous. See our article on *Surface Plasmon Polaritons* where the latter continuity requirement is essential.

---

[20] This is just one of many forms.

4.7.3 Graded Index Waveguides

Think of a substrate like glass or lithium niobate. Its surface may be treated by various processes in order to modify the permittivity at the surface, such as in-diffusion or exchange of ions. Lithium niobate may be covered by a thin titanium layer which is then allowed to diffuse into the substrate at high temperatures. Another procedure is to apply benzoic acid which replaces a certain amount of lithium ions by protons. With glass, one can offer silver ions which are drawn into the substrate by an electric field.

In any case, a permittivity profile is produced which exceeds the substrate value by $\Delta\epsilon(x)$, where x is the depth below the surface at $x = 0$. The region $x < 0$ is the cover, usually vacuum or air, or a protective substance. Its permittivity is denoted by ϵ_c. The substrate permittivity ϵ_s is larger than ϵ_c. Since the concentration of in-diffused ions follows a Gaussian and since, for not too high concentrations, the permittivity change is proportional to the concentration of in-diffused ions, we assume

$$\epsilon(x) = \begin{cases} \epsilon_\text{c} \text{ for } x < 0 \\ \epsilon_\text{s} + \Delta\epsilon\, \text{e}^{-(x/w)^2} \text{ for } x > 0 \end{cases}. \tag{4.166}$$

w denotes the width of the permittivity increase, and $\Delta\epsilon$ the maximum permittivity enhancement. Equation (4.166) is a rather good approximation for titanium in-diffused planar waveguides.

The standard procedure to solve such an eigenvalue problem is to approximate the infinite x axis $\mathbb{R}$ by a finite number $x_j = x_\text{min}, x_\text{min} + h, \dots, x_\text{max}$ of representative points. The field values $F_j = F(x_j)$ form a vector. A linear operator is represented by a square matrix. Here we describe the method of finite differences: infinitesimals dx are approximated by finite differences, h in our cases. The second derivative in particular is represented by

$$f''(x_j) = f_j'' = \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}, \tag{4.167}$$

which can be translated into a matrix to be applied to a vector f. This matrix has a diagonal $-2/h^2$ and adjacent diagonals $1/h^2$. A multiplication operator, such as $f \to \epsilon f$ is represented by a diagonal matrix with elements $\epsilon_j = \epsilon(x_j)$.

Here is a realization.

Our `MATLAB` program begins by defining constants. All lengths are measured in microns.

```
LAMBDA=0.6328;
k0=2*pi/LAMBDA;
EC=1.000;
ES=4.800;
ED=0.045;
W=4.00;
```

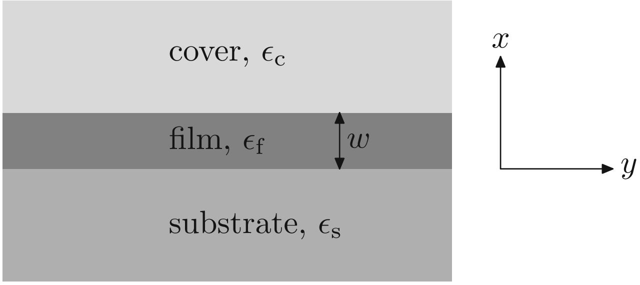

Fig. 4.7 Layout of a slab waveguide with one film of enhanced permittivity

The wavelength is that of a helium-neon laser, the cover is air, the substrate permittivity is that of lithium niobate, and the permittivity profile parameters $\Delta\epsilon$ (`ED`) and W are realistic.

We next represent the real axis by a finite set of representative values. They run from -1 to $4W$, in steps of h.

```
xmin=-1.0;
xmax=4*W;
h=0.1;
x=(xmin:h:xmax)';
dim=size(x,1);
```

The next line defines the permittivity profile:

```
prm=(x<0).*EC+(x>=0).*(ES+ED*exp(-(x/W).^2));
```

The following piece of code sets up the mode operator L:

```
next=ones(dim-1,1)/h^2/k0^2;
main=-2.0*ones(dim,1)/h^2/k0^2+prm;
L=diag(next,-1)+diag(main,0)+diag(next,1);
```

Its eigenvectors and eigenvalues are calculated by

```
[evec, eval]=eig(L);
```

Only eigenvectors with eigenvalues $(\beta/k_0)^2 = \epsilon_{\text{eff}} > \epsilon_s$ make sense. We isolate and plot them:

```
eff_eps=diag(eval);
guided=evec(:,eff_eps>ES);
plot(x,guided);
```

Figure 4.7 shows the output. There are three guided TE modes which are indexed by TE0, TE1, and TE2. The lowest order mode, the one with the largest propagation constant, has no node. The next one has one node, and so forth.

4.7.4 Slab Waveguides

A slab waveguide is made up of a substrate carrying one ore more homogeneous films of enhanced permittivity. On top is a cover layer. Here we study a very simple device. There is just one film with permittivity $\epsilon_\mathrm{f} > \epsilon_\mathrm{s}$ of thickness w. The permittivity profile is

$$\epsilon(x) = \begin{cases} \epsilon_\mathrm{s} \text{ for } x < 0 \\ \epsilon_\mathrm{f} \text{ for } 0 < x < w \\ \epsilon_\mathrm{c} \text{ for } w < x \end{cases} . \tag{4.168}$$

Formally, the TE and the TM mode operators, (4.161) and (4.165) respectively, coincide for such a stepwise constant profile. However since the continuity requirements differ, the propagation constants and the modal fields are different for TE and TM modes.

Let us define

$$\kappa_\mathrm{c} = k_0\sqrt{\epsilon_\mathrm{eff} - \epsilon_\mathrm{c}}\ ,\ \kappa_\mathrm{s} = k_0\sqrt{\epsilon_\mathrm{eff} - \epsilon_\mathrm{s}} \text{ and } k_\mathrm{f} = k_0\sqrt{\epsilon_\mathrm{f} - \epsilon_\mathrm{eff}}. \tag{4.169}$$

These expressions are positive as long as we insist on $\epsilon_\mathrm{c}, \epsilon_\mathrm{s} < \epsilon_\mathrm{eff} < \epsilon_\mathrm{f}$.

In the substrate region, the mode equation has two fundamental solutions, namely $E \propto \exp(\pm\kappa_\mathrm{s} x)$. We choose the positive sign in order to guarantee decay at $x \to -\infty$.

For the TE mode, the field and its derivative have to be continuous at interfaces between different materials. The solutions in the film region is $c\cos(k_\mathrm{f} x) + s\sin(k_\mathrm{f} x)$. We therefore have to determine the amplitudes c and s such that

$$1 = c \text{ and } \kappa_\mathrm{s} = s k_\mathrm{f} \tag{4.170}$$

hold true at the interface $x = 0$ between substrate and film. Therefore

$$E \propto \cos k_\mathrm{f} x + \frac{\kappa_\mathrm{s}}{k_\mathrm{f}} \sin k_\mathrm{f} x \text{ for } 0 < x < w. \tag{4.171}$$

In the cover $x > w$ the field is a linear combination of two exponential functions, namely $E \propto a\exp(-\kappa_\mathrm{c} x) + b\exp(-\kappa_\mathrm{c} x)$. The continuity requirements for TE modes at $x = w$ are

$$\cos k_\mathrm{f} w + \frac{\kappa_\mathrm{s}}{k_\mathrm{f}} \sin k_\mathrm{f} w = a\,\mathrm{e}^{-\kappa_\mathrm{c} w} + b\,\mathrm{e}^{\kappa_\mathrm{c} w} \tag{4.172}$$

and

$$k_\mathrm{f}\left(-\sin k_\mathrm{f} w + \frac{\kappa_\mathrm{s}}{k_\mathrm{f}} \cos k_\mathrm{f} w\right) = \kappa_\mathrm{c}\left(-a\,\mathrm{e}^{-\kappa_\mathrm{c} w} + b\,\mathrm{e}^{\kappa_\mathrm{c} w}\right). \tag{4.173}$$

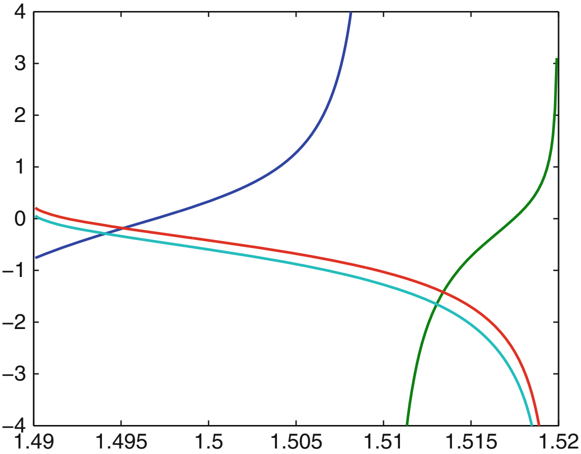

Fig. 4.8 Graphical representation of Eqs. (4.174) and (4.175). The cotangent as well as the *right hand sides* are plotted vs. effective index $n_{\text{eff}} = \sqrt{\epsilon_{\text{eff}}}$. The *upper curve* corresponds to TE, the *lower* to TM polarization. The film (refractive index 1.52, thickness 1.8 µm) is deposited on a glass substrate (refractive index 1.49) and covered by air. The simulation is for a helium-neon laser. There are two guided TE and two guided TM modes

The condition for a guided mode reads $b = 0$. There must not be an exploding contribution. Equations (4.172) and (4.173) are compatible only if

$$\cot k_{\text{f}} w = \frac{k_{\text{f}}^2 - \kappa_{\text{s}} \kappa_{\text{c}}}{k_{\text{f}} (\kappa_{\text{s}} + \kappa_{\text{c}})} \tag{4.174}$$

holds true.

An analogous calculation for TM modes results in

$$\cot k_{\text{f}} w = \frac{\bar{k}_{\text{f}}^2 - \bar{\kappa}_{\text{s}} \bar{\kappa}_{\text{c}}}{\bar{k}_{\text{f}} (\bar{\kappa}_{\text{s}} + \bar{\kappa}_{\text{c}})} \tag{4.175}$$

where $\bar{\kappa}_{\text{c}} = \kappa_{\text{c}} / \epsilon_{\text{c}}$, $\bar{\kappa}_{\text{s}} = \kappa_{\text{s}} / \epsilon_{\text{s}}$ and $\bar{k}_{\text{f}} = k_{\text{f}} / \epsilon_{\text{f}}$ (Fig. 4.8).

Note that the right hand side of Eq. (4.175) is smaller than its TE counterpart. Therefore, the propagation constants of TM modes are smaller than the corresponding TE values.

Formulas (4.174) or (4.175) allow for an inverse procedure. Assume that at least two TE modes are guided. One can then, for a guessed film refractive index n_{f}, solve Eq. (4.174) for the film thickness w. For each mode i, a film thickness w_i results, but they will coincide only if the guessed film refractive index is correct. If there are more than two modes, the root mean square deviation of calculated film thicknesses must be minimized. Applying the same procedure to TM modes should result in the same film parameters.

4.8 Elasticity Moduli

We repeat that this small book on continuum physics cannot really cover such a vast field. Instead we try to formulate the foundation—balance equations—and to characterize entire fields of physics and engineering by material equations. We have also introduced a systematic way to derive macroscopic laws from quantum statistical mechanics by working out the linear response to perturbations. The fourth part is a collection of seemingly randomly chosen examples to make the reader acquainted with applications. Such as this, where we comment on some standard problems of elasticity theory.

4.8.1 Strain and Stress

We have introduced in the section on *Solid Media* a framework how to describe the deformation and the stress of a solid body. A particular material point, originally at $\boldsymbol{x}$, is translated to $\bar{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{u}$, where $\boldsymbol{u} = \boldsymbol{u}(t, \boldsymbol{x})$ is the displacement field. The strain tensor is

$$S_{ij} = \frac{\partial_i u_j + \partial_j u_i}{2}\,, \tag{4.176}$$

it will vanish if the solid is translated or rotated as a whole. Hence, the strain really describes the deformation of the solid such that distances between material points will change.

Also recall that the momentum current $j_i(P_k)$ consists of the convection part $\varrho v_i v_k$ and the conduction term $J_i(P_k) = -T_{ik}$. Here P_k are the three components of linear momentum, ϱ is the mass density and v_i denotes the flow velocity. The stress tensor T_{ik} is symmetric. It consists of an elastic contribution T'_{ik}, which transforms like the convection part, and an inelastic contribution T''_{ik} which is odd under time reversal and describes friction.

Structural mechanics is concerned with the stability and optimization of mechanical structures like bridges, houses, dams, cars, ship and airplanes, and so forth. The structure itself can mostly be assumed at rest. See however the section on *Bulk and Surface Acoustic Waves in Solids*. So there is no change with time, no flow, and no friction. We have to solve the momentum balance equation

$$\partial_i T_{ik} + f_k = 0, \tag{4.177}$$

where f_k is the external force per unit volume. There can be gravitation or a fictitious, or pseudo force, for example due to rotation.

If there is no stress, there will be no strain. Hence, a linear relationship between stress and strain, Hooke's law, is to be expected.

4.8.2 Uniaxial Stress

Consider a homogeneous straight square column of height h and cross section $q \times q$. The column bottom is fixed on a rigid platform, the top is drawn at by a force σq^2. σ, as a force per unit area, is the equally distributed stress exerted on the top of the column.

The height of this column is increased to $h + \delta h$, and δh will be proportional to h and to the stress. We express this finding by

$$\frac{\delta h}{h} = \frac{\sigma}{E}. \tag{4.178}$$

The constant E is called the elasticity, or Young's modulus. Its dimension is force per area, i.e., Newton per square meter.

The column becomes not only longer, but also thinner. Its lateral dimension changes from q to $q - \delta q$, and δq will be proportional to q and σ. In the usual notation this reads

$$\frac{\delta q}{q} = \nu \frac{\sigma}{E}. \tag{4.179}$$

The dimensionless number ν is Poisson's ratio.

Young's modulus and Poisson's ratio have been introduced formally in the chapter on *Material Equations*, here we have given a practical definition.

The deformation of the elastic body can be described by the following displacement field:

$$\boldsymbol{u}(\boldsymbol{x}) = \begin{pmatrix} -\delta q x_1/q \\ -\delta q x_2/q \\ \delta h x_3/h \end{pmatrix}, \tag{4.180}$$

for a column $-q/2 \le x1, x_2 \le q/2$ and $0 \le x_3 \le h$. The resulting strain tensor is

$$S_{ij} = \begin{pmatrix} -\delta q/q & 0 & 0 \\ 0 & -\delta q/q & 0 \\ 0 & 0 & \delta h/h \end{pmatrix}. \tag{4.181}$$

With Hooke's law (2.38) for an isotropic medium, namely

$$T_{ij} = \frac{E}{1+\nu}\left\{S_{ij} + \frac{\nu}{1-2\nu}\delta_{ij} S_{kk}\right\} \tag{4.182}$$

and with Eqs. (4.178), (4.179) and (4.181) one easily works out

$$T_{33} = \sigma \tag{4.183}$$

and vanishes otherwise. This says that only the momentum component P_3 flows, namely in 3-direction, and that its magnitude is σ. This was to be expected.

Obviously the problem has been solved. An external force does not come into play, the divergence $\partial_i T_{ij}$ vanishes, and stress is related with strain in such a way that the latter can be derived from a displacement field.

Note that the stress tensor is already diagonal and that two of its eigenvalues vanish. In this case one speaks of uniaxial stress. Also note that Eq. (4.183) is valid for a column of arbitrary cross section.

4.8.3 Hydrostatic Pressure

Assume a homogeneous elastic body of arbitrary shape immersed in a liquid of constant pressure p. Outside, the stress tensor is $T_{ij} = -p\delta_{ij}$ because the medium is fluid and cannot support shear forces. Inside, in the elastic medium, the stress tensor is also $T_{ij} = -p\delta_{ij}$ although the material could support shear forces. After all, the stress tensor is a momentum current which must be continuous at the boundary.

The relation between stress and strain is Eq. (4.183) or its inverse

$$S_{ij} = \frac{1+\nu}{E} T_{ij} - \frac{\nu}{E} \delta_{ij} T_{kk}, \tag{4.184}$$

see Eq. (2.35). In our case this means

$$S_{ij} = -\frac{1-2\nu}{E} p\delta_{ij}. \tag{4.185}$$

The strain tensor can be derived from a displacement field

$$S_{ij} = \frac{\partial_i u_j + \partial_j u_i}{2} \text{ where } \boldsymbol{u}(\boldsymbol{x}) = -p\frac{1-2\nu}{E}\boldsymbol{x}. \tag{4.186}$$

We have chosen $\boldsymbol{x}_0 = 0$ as a reference point within the elastic body, its center of mass position, for example.

With $\boldsymbol{n}$, a unit vector, we may write $\boldsymbol{x} = r\boldsymbol{n}$. The point $r\boldsymbol{n}$ is displaced to $(r - \delta r)\boldsymbol{n}$, and we have just calculated

$$3\frac{\delta r}{r} = \frac{\delta V}{V} = \frac{p}{K}, \tag{4.187}$$

where the so called compression modulus K is given by

$$K = \frac{E}{3(1-2\nu)}. \tag{4.188}$$

$\delta V/V$ is the relative volume change.

4.8.4 Torsion

Think about a circular rod of diameter $2R$ and length ℓ. The rod is fixed at the bottom while the top is twisted by an angle α. Each slab of this rod will be twisted by an angle $\alpha x_3/\ell$ which grows linearly with height x_3. The corresponding displacement field is

$$\boldsymbol{u}(\boldsymbol{x}) = \begin{pmatrix} \cos(\gamma x_3)x_1 - \sin(\gamma x_3)x_2 - x_1 \\ \sin(\gamma x_3)x_1 + \cos(\gamma x_3)x_2 - x_2 \\ 0 \end{pmatrix}. \tag{4.189}$$

$\gamma = \alpha/L$ is the twist, or torsion angle per unit length. Since it is small, we may write the displacement field as

$$u_1 = -\gamma x_2 x_3 \, , \, u_2 = +\gamma x_1 x_3 \, , \, u_3 = 0. \tag{4.190}$$

This expression leads to the following strain tensor:

$$S_{ij} = \frac{\gamma}{2} \begin{pmatrix} 0 & 0 & -x_2 \\ 0 & 0 & x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}. \tag{4.191}$$

Recall formula (2.33) which says that the relative change of volume elements is equal to the trace of the strain tensor:

$$\frac{\mathrm{d}\bar{V} - \mathrm{d}V}{V} = S_{kk}. \tag{4.192}$$

We conclude that the volume elements do not change if torsion is applied to an elastic body, i.e., if it is sheared.

The strain (4.192) is related to a stress tensor

$$T_{ij} = \frac{\gamma E}{2(1+\nu)} \begin{pmatrix} 0 & 0 & -x_2 \\ 0 & 0 & x_1 \\ -x_2 & x_1 & 0 \end{pmatrix}. \tag{4.193}$$

You may easily verify that $\partial_i T_{ij} = 0$ holds true, that the equation for mechanical equilibrium is satisfied.

Let us calculate the torque on the entire cross section:

$$N = \int\limits_{x_1^2+x_2^2\le R^2} \mathrm{d}x_1 \mathrm{d}x_2 \, (x_1 T_{23} - x_2 T_{13}) = \frac{\gamma E}{2(1+\nu)} \frac{\pi R^4}{2}. \tag{4.194}$$

Our result may be reformulated as

$$\frac{\alpha}{\ell} = \frac{1}{G}\frac{N}{I}, \tag{4.195}$$

where N is the torque by which the rod is twisted, I the area moment, and G the shear modulus. The latter is defined as

$$G = \frac{E}{2(1+\nu)}. \tag{4.196}$$

The area moment is an integral over the cross section, namely

$$I = I_x + I_y = \int \mathrm{d}A\,(x_1^2 + x_2^2). \tag{4.197}$$

For a solid rod of radius R it is given by $\pi R^4/2$, but Eq. (4.195) holds true for arbitrary cross sections. See article *Beam Bending and Buckling*.

4.8.5 Examples: Steel and Rubber

The elasticity modulus of true solids is a microscopic property of bulk matter. Its physical dimension is a pressure, or an energy density. We therefore expect values of the order of $\mathrm{eV}/\text{Å}^3 = 160\,\mathrm{GPa}$.

In fact, the value for stainless steel [5] at room temperature is about $E = 215\,\mathrm{GPa}$, varying slightly according to composition. Poisson's ratio turns out to be about $\nu = 0.29$. A value around 0.3 is typical for metals.

However, the decisive quantity in most application is not the elasticity modulus, but the so called yield stress. If one of the three eigenvalues of the stress tensor, at any place, exceeds this value, the medium looses its elastic properties. In contrast to the elasticity modulus or Poisson's ratio, the yield stress is a consequence of material imperfections, such as dislocations of all kind. As a rule of thumb, the yield stress is three orders of magnitude smaller than the elasticity modulus. For example, the yield stresses of the many brands of steel may vary from 0.28 to 1.6 GPa.

In 1839 Charles Goodyear invented a method how to transform plastic caoutchouc into elastic rubber. Caoutchouc is made from latex, a milky substance collected from tapped rubber trees. With the advance of the automobile, rubber was much needed for tires which gave rise to brutal exploitation of the Amazon and the Congo region and, less brutally, of Ceylon where the rubber trees could be grown in plantations. Today the larger part of rubber is produced synthetically.

Rubber almost behaves as a liquid which retains its volume but may be deformed without much effort. The elasticity modulus practically vanishes. Indeed, Poisson's ratio for rubber is close to 1/2, and $K = 10\,\mathrm{GPa}$ is a typical value for the compression modulus.

However, rubber-like materials are a class of its own because they can be deformed to such an extent that the approximation $2S_{ij} = \partial_i u_j + \partial_j u_i + \dots$ is no longer justified. Unfortunately, we cannot delve into more details here.

4.9 Faraday Effect

In 1845 Michael Faraday discovered that a magnetic field may affect the propagation of light. This was a strong indication that light is an electromagnetic phenomenon, as was proven shortly afterwards by James Clark Maxwell in his famous *Treatise on Electricity and Magnetism*. In this article we study the contribution to the susceptibility by a quasi-static external or internal magnetic field and its effect on light propagation. We comment on the reciprocity theorem of signal processing devices and show that only the linear magnetooptic effect allows isolators which are essential for laser driven glass fiber communication lines. To realize an integrated magnetooptical isolator with micrometer dimensions is an ongoing effort.

4.9.1 Susceptibility and Onsager's Relation

If a medium is perturbed by an electric field, it becomes polarized. For sufficiently small field strength, the response (polarization) depends linearly on the perturbation (electric field strength). The most general linear and causal dependency is described by

$$P_i(t,\boldsymbol{x}) = \int_0^\infty \mathrm{d}t \int \mathrm{d}^3\xi \, \Gamma_{ij}(\tau,\boldsymbol{\xi}) \, E_j(t-\tau,\boldsymbol{x}-\boldsymbol{\xi}). \tag{4.198}$$

Fourier transforming this results in[21]

$$\tilde{P}_i(\omega,\boldsymbol{k}) = \epsilon_0 \chi_{ij}(\omega,\boldsymbol{k}) \, \tilde{E}_j(\omega,\boldsymbol{k}). \tag{4.199}$$

Because the speed of light is so much larger than the speed of sound in a solid or liquid, only $\boldsymbol{k} = 0$ is of interest in optics.[22] The susceptibility tensor is an expectation value in the Gibbs state. It depends on all parameters which characterize the thermodynamic equilibrium. Static or slowly varying electric or magnetic fields are examples.

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[21] Later on we drop the tilde as indicator of a Fourier component.

[22] *Optical activity* is an exception.

We here discuss a transparent material which is characterized by a Hermitian susceptibility tensor,[23] $\chi_{ij} = \chi^*_{ji}$. Onsager's relation states that χ_{ij} for $\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}$ is the same as χ_{ji} for $\boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}$. The same holds true for the permittivity tensor ϵ_{ij} or its inverse $\epsilon^{-1}{}_{ij}$.

A power series expansion results in

$$\epsilon^{-1}{}_{ij} = \epsilon^{-1}{}^{(0,0)}_{ij} + \epsilon^{-1}{}^{(1,0)}_{ijk} \mathcal{E}_k + \epsilon^{-1}{}^{(0,1)}_{ijk} \mathcal{B}_k + \dots . \tag{4.200}$$

The first term on the right hand side of Eq. (4.200) is the dielectric permittivity without an external electric or magnetic field. We have studied it in the article on *Crystal Optics*. The second term describes the Pockels effect which is the main topic of our discourse on *Pockels and Kerr Effect*. In this article we are concerned with the third term which describes how a quasi-static magnetic field affects the propagation of light.

That the medium under study be transparent and Onsager's relation require that the first contribution is real and symmetric. For an optically isotropic medium we may write

$$\epsilon^{-1}{}^{(0,0)}_{ij} = \frac{1}{n^2} \delta_{ij} , \tag{4.201}$$

with a real refractive index n. The second contribution vanishes because no electric field is applied.

The third contribution Δ_{ij} must fulfill

- $\Delta_{ij} = \Delta^*_{ji}$ because the medium is transparent and
- $\Delta_{ij} = -\Delta_{ji}$ in order to comply with Onsager's relations.

Hence Δ_{ij} is purely imaginary and anti-symmetric. An obvious choice is $\Delta_{ij} = \mathrm{i}\kappa\epsilon_{ijk}\mathcal{B}_k$, with a real κ. Because this contribution will be small, it can be rewritten as

$$\epsilon_{ij} = n^2 \delta_{ij} + \mathrm{i}\, K \epsilon_{ijk} \mathcal{B}_k . \tag{4.202}$$

This formula describes the Faraday effect of an optically isotropic medium. $K = K(\omega)$ is a real number for a given frequency. Less symmetric media must be characterized by additional contributions.

4.9.2 Rotation of the Polarization Vector

Assume a transparent medium and a magnetic induction $\boldsymbol{\mathcal{B}} = (0, 0, \mathcal{B})$ in z-direction. The permittivity tensor will be

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[23] We drop the arguments $(\omega, \boldsymbol{k} = 0)$.

$$\epsilon = \begin{pmatrix} n^2 & \mathrm{i}K\mathcal{B} & 0 \\ -\mathrm{i}K\mathcal{B} & n^2 & 0 \\ 0 & 0 & n^2 \end{pmatrix}. \tag{4.203}$$

Beams traveling in the x, y-plane are polarized perpendicularly, in z-direction. They propagate as linearly polarized beams with propagation constant nk_0, where $k_0 = \omega/c$ is the wave vacuum wave number. They are not affected by the Faraday effect.

Let us now study a plane wave traveling along the z-axis, parallel to the magnetic field. We look for modes which propagate with a definite propagation constant β in z-direction,

$$\boldsymbol{E}(t, x, y, z) = A\,\hat{\boldsymbol{e}}\ \mathrm{e}^{-\mathrm{i}\omega t}\ \mathrm{e}^{\mathrm{i}\beta z}. \tag{4.204}$$

$\boldsymbol{E}$ is the electric field strength, A the amplitude, $\hat{\boldsymbol{e}}$ the polarization unit vector, ω the angular frequency and β the propagation constant, an inverse length. It is a plane wave since x and y do not show up on the right hand side of Eq. (4.204). As demonstrated in *Crystal optics*, the following eigenvalue equation has to be solved:

$$\epsilon_{ij}\hat{e}_j = \nu^2 \hat{e}_i, \tag{4.205}$$

where $\nu = \beta/k_0$.

The matrix ϵ of Eq. (4.203) has three real eigenvalues.

One is $\nu^2 = n^2$ with eigenvector $\hat{\boldsymbol{e}} = (0, 0, 1)$. We have already mentioned it. It corresponds to beams propagating in the x, y-plane. Their propagation constant is not affected by the quasi-static magnetic field.

The remaining two eigenvalues are

$$\nu^2 = n^2 \pm K\mathcal{B} \text{ or } \nu_{\pm} = \sqrt{n^2 \pm K\mathcal{B}} = n \pm \frac{K\mathcal{B}}{2n}. \tag{4.206}$$

The corresponding normalized eigenvectors are

$$\hat{\boldsymbol{e}}_{+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \\ 0 \end{pmatrix} \text{ and } \hat{\boldsymbol{e}}_{-} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ +\mathrm{i} \\ 0 \end{pmatrix}. \tag{4.207}$$

They describe circularly polarized waves, because the polarization vector

$$\mathrm{Re}\, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp\mathrm{i} \\ 0 \end{pmatrix} \mathrm{e}^{-\mathrm{i}\omega t}\ \mathrm{e}^{\mathrm{i}\beta_{\pm} z} = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(\omega t - \beta_{\pm} z) \\ \mp \sin(\omega t - \beta_{\pm} z) \\ 0 \end{pmatrix} \tag{4.208}$$

rotates on a circle in the x, y-plane. For fixed time, this is a helix, either left- or right handed. For fixed location, the polarization vector rotates clock- or anticlock-wise, respectively.

Assume that a linearly polarized beam enters the medium at $z = 0$. Its polarization vector

$$\hat{\boldsymbol{e}}_x = \frac{1}{\sqrt{2}}\hat{\boldsymbol{e}}_+ + \frac{1}{\sqrt{2}}\hat{\boldsymbol{e}}_- \tag{4.209}$$

say, is a superposition of left- and right-handed polarization. Having traveled the distance ℓ with slightly different propagation constants, the polarization vector has become

$$\frac{1}{\sqrt{2}}\hat{\boldsymbol{e}}_+\,\mathrm{e}^{\,\mathrm{i}K\mathcal{B}k_0\ell/2n} + \frac{1}{\sqrt{2}}\hat{\boldsymbol{e}}_-\,\mathrm{e}^{\,-\mathrm{i}K\mathcal{B}k_0\ell/2n} = \begin{pmatrix}\cos\Phi^{\mathrm{F}}\ell\\ \sin\Phi^{\mathrm{F}}\ell\\ 0\end{pmatrix}. \tag{4.210}$$

The polarization is again linear, but it has been rotated by the angle $\ell\,\Phi^{\mathrm{F}}$ where

$$\Phi^{\mathrm{F}} = \frac{K\mathcal{B}k_0}{2n} = \pi\frac{K\mathcal{B}}{n\lambda_0} = \mathcal{V}\mathcal{B}. \tag{4.211}$$

Φ^{F} is the specific[24] Faraday rotation. λ_0 stands for the vacuum wave length $\omega c/2\pi$. $\mathcal{V}$ is known as Verdet's constant.

The Verdet constant of water under standard conditions is listed in [5] as $1.65 \times 10^{-2}\,\mathrm{min\,A}^{-1}$. This value obviously refers to the magnetic field strength $\mathcal{H}$ which is measured in A/m. Replacing the minute by $2\pi/(360 \times 60)$ and $\mathcal{H}$ by $\mathcal{B} = \mu_0\mathcal{H}$, we arrive at $\mathcal{V} = 3.82\ \mathrm{T}^{-1}\,\mathrm{m}^{-1}$.

4.9.3 Drude Model

Assume an isolator and think of a typical valence electron. Its deviation $\boldsymbol{x}$ from the equilibrium position obeys the following equation of motion:

$$m\{\ddot{\boldsymbol{x}} + \Gamma\dot{\boldsymbol{x}} + \Omega^2\boldsymbol{x}\} = -e\boldsymbol{E}(t) - e\dot{\boldsymbol{x}} \times \boldsymbol{\mathcal{B}}. \tag{4.212}$$

m is the electron mass, Γ describes friction, and $m\Omega^2$ is the spring constant. On the right hand side you find the rapidly oscillation electric field $\boldsymbol{E}$ of a light wave and a quasi-static induction field $\boldsymbol{\mathcal{B}}$. They drive the electron's motion. Compare this *ansatz* with Eq. (4.463) in the article on *Surface Plasmon Polaritons* in which we derived an expression for the permittivity $\epsilon = \epsilon(\omega)$ of a noble metal. There we had to deal with a gas of quasi-free electrons ($\Omega = 0$), and there was no external induction field.

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[24] In this context: per unit length.

Assume that the induction points along the z-direction and that the light wave oscillates with angular frequency ω and is clockwise circularly polarized. We write

$$\boldsymbol{E} = E\,\mathrm{e}^{-\mathrm{i}\omega t}\,\hat{\boldsymbol{e}}_+\,,\ \boldsymbol{\mathcal{B}} = \mathcal{B}\hat{\boldsymbol{e}}_z \text{ and } \boldsymbol{x} = x\,\mathrm{e}^{-\mathrm{i}\omega t}\,\hat{\boldsymbol{e}}_+. \tag{4.213}$$

Because of $\dot{\boldsymbol{x}} \times \boldsymbol{\mathcal{B}} = -\omega x \mathcal{B}\hat{\boldsymbol{e}}_+$, Eq. (4.212) reduces to

$$m\{-\omega^2 - \mathrm{i}\Gamma\omega + \Omega^2\}x = -eE + e\omega\mathcal{B}x, \tag{4.214}$$

the solution of which is

$$x = \frac{-eE}{m(\omega^2 - \Omega^2) + e\omega\mathcal{B} + \mathrm{i}m\omega\Gamma}. \tag{4.215}$$

There are N such typical electrons per unit volume, each contributing with $-ex$ to the polarization. The ratio of polarization to electric field strength gives the susceptibility

$$\chi_\pm = \frac{e^2 N}{\epsilon_0}\,\frac{1}{m(\omega^2 - \Omega^2) \pm e\omega\mathcal{B} + \mathrm{i}m\omega\Gamma}. \tag{4.216}$$

We have already anticipated that the calculation for an anti-clockwise circularly polarized light wave leads to a minus sign in the $\mathcal{B}$ term.

The Drude model may be criticized for many reasons:

- It does not take quantum effects into account.[25] Indeed, $\hbar$ is missing in Eq. (4.216).
- There is not just one resonance frequency Ω, but a distribution thereof. This can be remedied.
- The differences between electric conductors, semi-conductors, insulators, solids, liquids, gases, ferro- and ferrimagnetic substances are ignored.
- and many more objections.

Nevertheless, we have presented the Drude model here in order to show that an externally applied magnetic induction indeed affects the propagation of left- or right handed light. Even if the Drude model is too primitive to be taken seriously, it shows that there *must* be a Faraday effect. After all, the electric field $\boldsymbol{E}$ of a light wave affects electrons, in the presence of a quasi-static induction, by a force $-e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{\mathcal{B}})$. Irrespective of how this is translated into susceptibilities, both contributions come together.

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[25] At least only indirectly, because n, Γ and Ω have to be calculated within the framework of quantum mechanics. Even for quasi-free electrons, m is the effective mass an expression which depends explicitly on $\hbar$.

4.9.4 Optical Isolator

If a linearly polarized beam passes through a medium in direction of an induction field, its polarization remains linear. However, this polarization vector becomes rotated clockwise[26] by an amount which is proportional to the thickness of the sample. Now, if this beam is reflected and runs through the medium in opposite direction, the polarization vector again becomes rotated, and again clockwise. The rotation is not undone upon reflection. We will comment on this peculiar finding later.

The Faraday effect allows to build an optical isolator, a device that is transparent in forward direction, while it blocks light in backward direction. You need a polarizer oriented such that only $\hat{\boldsymbol{e}}_y$ polarized light may pass. Then, there is a Faraday rotator which produces a 45° rotation of the polarization vector. A second polarizer, rotated by 45° with respect to the first, allows all light to pass on.

Now, if a reflected light beam enters the device in opposite direction, the second polarizer transmits only that part which is linearly polarized at 45°. The Faraday rotator changes this angle to 90°, and the first polarizer blocks such light which is polarized along $\hat{\boldsymbol{e}}_x$.

The transmission factor in backward direction vanishes ideally. The transmission factor in forward direction varies from zero (the incoming light is linearly polarized in $\hat{\boldsymbol{e}}_x$ direction) to one (the incoming light is linearly polarized in $\hat{\boldsymbol{e}}_y$ direction). For unpolarized light the transmission factor in forward direction is one half.

Reversing the propagation direction of a light beam is the same as time reversal. Maxwell's equations respect time reversal. How can forward and backward propagation of light be different? After all, there is the so-called reciprocity theorem of electrical engineering. It says that any linear device with channels $i = 1, 2\dots$ behaves as $O_i = \sum_j D_{ij} I_j$ where O_i is the output at channel i and I_j the input at channel j, and that D is a symmetric matrix. That is, reversing the nature of emitters and receivers is a symmetry. Broadcasting at A and receiving at B weakens the signal by the same amount as if the same broadcasting station were situated at B and the signal received at A. In this context, an optical isolator seems to be impossible. Let us study details.

Time inversion is described by $(t, \boldsymbol{x}) \to (-t, \boldsymbol{x})$. With

$$\{\varrho', \boldsymbol{j}', \boldsymbol{E}', \boldsymbol{B}'\}(t, \boldsymbol{x}) = \{\varrho, -\boldsymbol{j}, \boldsymbol{E}, -\boldsymbol{B}\}(-t, \boldsymbol{x}) \tag{4.217}$$

the primed fields obey Maxwell's equations if the unprimed do so. Equation (4.217) is the base of the reciprocity theorem mentioned above. Note that the Pointing vector $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ changes sign upon time reversal.

If applied to the optical isolator, the *entire* magnetic field should be reversed. The rapidly oscillation induction field $\boldsymbol{B}$ of the light wave indeed changes sign

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[26] We assume a positive Verdet constant.

upon reflection, but not the quasi-static field $\mathcal{B}$ of the Faraday rotator, it remains unchanged. A device like an optical isolator or circulator cannot be realized without materials which have a preferred magnetic axis. This preference can be induced by applying an external field, or it may be inherent.

4.9.5 Yttrium Iron Garnet

A quasi-static external magnetic field is rather impracticable. Much better are materials with an inherent magnetic field such as ferro- or ferrimagnets. However, most ferromagnetic materials, such as iron, are electric conductors which strongly absorb light. Yttrium iron garnet, $Y_3Fe_2(FeO_4)_3$, is an artificial ferrimagnetic crystal which is transparent in the near infrared.[27] The specific Faraday rotation of yttrium iron garnet (YIG) can be manipulated by doping with or substitution of ions. In particular, the addition of bismuth or cerium proves to be rather efficient. For integrated optics applications, thin YIG films are grown by liquid phase epitaxy on gadolinium gallium garnets (GGG). The mismatch of lattice constants produces strong stresses in the films which cause birefringence in the otherwise optically isotropic garnets. Specific Faraday rotation constants up to −500 degrees per millimeter have been reported. This makes an integrated optical isolator of sub-millimeter length a feasible device.

4.10 Fourier's Solution of a Heat Conduction Problem

Joseph Fourier, while being prefect of the Département Isère at Grenoble, had soon complied with his few official duties. He then spent his time by studying the propagation of heat. The fruit of these studies, the book *Théorie analytique de la chaleur*, is considered to be one of the classics of physics because he introduced a new mathematical technique: decomposing periodic functions into a series of sine and cosine functions.

The problem to be solved is the following. Denote by $T = T(t, x)$ the temperature at time t at a depth x below the surface. $T_0(t) = T(t, 0)$ is prescribed, it is a periodic function with period τ which may be 1 day or 1 year. Find the solution of

$$\frac{\partial T}{\partial t} = \kappa \, \frac{\partial^2 T}{\partial x^2}, \tag{4.218}$$

with constant thermal diffusivity. $\kappa = 1 \times 10^{-7}\,\mathrm{m}^2\,\mathrm{s}^{-1}$ is a typical value. We here present Fourier's masterpiece in modern notation.

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[27] Glass fibers have minimal absorption losses at $\lambda = 1.50\,\mu\mathrm{m}$.

4.10.1 Representation of a Periodic Function

Since the boundary condition at $t = 0$ is periodic, the solution will be periodic as well. Therefore we write

$$T(t,x) = \sum_{k\in\mathbb{Z}} \mathrm{e}^{\,2\pi \mathrm{i} k t/\tau}\,\theta_k(x) \tag{4.219}$$

which guarantees $T(t+\tau, x) = T(t, x)$. The sum runs over all integer numbers k. Note $\theta_{-k} = \theta_k^*$ because the temperature field is real. In what follows we assume that indexes k are non-negative.

We insert Eq. (4.219) into the heat equation (4.218) and obtain

$$\frac{2\pi \mathrm{i} k}{\tau}\theta_k(x) = \kappa \theta_k''(x). \tag{4.220}$$

These ordinary differential equations can be solved analytically.

4.10.2 Ordinary Instead of Partial Differential Equations

Because its coefficients are constant, an exponential function is appropriate,

$$\theta_k(x) \propto \mathrm{e}^{\,\Lambda_k x}\,. \tag{4.221}$$

We easily arrive at

$$\Lambda_k = \pm\sqrt{\frac{2\pi \mathrm{i} k}{\kappa\tau}} = \pm(1+\mathrm{i})\sqrt{\frac{\pi k}{\kappa\tau}}. \tag{4.222}$$

We must choose the minus sign in order to exclude exploding solutions. Hence

$$\theta_k(x) = \theta_k(0)\,\mathrm{e}^{\,-(1+\mathrm{i})\sqrt{\pi k/\kappa\tau}\,x}\,. \tag{4.223}$$

4.10.3 Initial Conditions

What remains is to determine the values $\theta_k(0)$. Recall that

$$T(t,0) = T_0(t) + \sum_{k\in\mathbb{Z}} \mathrm{e}^{\,2\pi \mathrm{i} k t/\tau}\,\theta_k(0) \tag{4.224}$$

is prescribed. We simply work out

$$\frac{1}{\tau}\int_0^\tau \mathrm{d}t\ \mathrm{e}^{-2\pi\mathrm{i}kt/\tau}\,T_0(t) = \theta_k(0), \tag{4.225}$$

because of

$$\frac{1}{\tau}\int_0^\tau \mathrm{d}t\ \mathrm{e}^{-2\pi\mathrm{i}(k-j)t/\tau} = \delta_{kj}. \tag{4.226}$$

The contribution for $k = 0$ is just the average surface temperature $\bar{T}$ which coincides with the constant temperature at large depth. With $\theta_{-k} = \theta_k^*$ we finally arrive at

$$T(t,x) = \bar{T} + 2\sum_{k=1}^{\infty} \mathrm{e}^{-q_k x}\ \mathrm{Re}\ \theta_k(0)\,\mathrm{e}^{2\pi\mathrm{i}kt/\tau}\ \mathrm{e}^{-\mathrm{i}q_k x}, \tag{4.227}$$

where

$$q_k = \sqrt{\pi k/\kappa\tau}. \tag{4.228}$$

Re denotes the real part of the expression right to it.

Temperature changes decay exponentially with increasing depth x. q_k is the attenuation constant of the kth Fourier component. Note the depth dependent phase shift, i.e., the last factor in Eq. (4.227).

With $\kappa \approx 1 \times 10^{-7}\,\mathrm{m}^2\,\mathrm{s}^{-1}$ and $\tau = 1$ year we find $q_1 \approx 1\ \mathrm{m}^{-1}$. So, the yearly temperature changes affect only a few meters beneath the surface.

Fourier's invention to decompose periodic functions into harmonics and to solve the heat equation for each harmonic contribution initiated a substantial progress of theoretical physics. Therefore, we should be grateful that a competent governor of a French province was left enough spare time to pursue his hobby.

4.11 Hagen-Poiseuille Law

The laminar flow of a viscous liquid through a straight pipe of circular cross section—this is a classic of hydrodynamics. The solution seems to be straightforward, simple and plausible, but can it be trusted? Quite ironically, the relationship between pressure, flux and pipe diameter was derived independently by a civil engineer and a physician for problems which cannot be idealized as laminar flow.

4.11.1 Exploiting Symmetry

We discuss a circular straight tube with interior diameter $2R$. The cross section is parameterized by x_1, x_2 and the direction of flow by $z = x_3$. The tube shall be very long so that the velocity field will not depend on z. Thus one may write

$$v_1 = v_2 = 0 \text{ and } v_3 = f(r) \tag{4.229}$$

where $r = \sqrt{x_1^2 + x_2^2}$.

The divergence $\partial_j v_j$ vanishes because v_1 and v_2 vanish and because v_3 does not depend on x_3. With Eq. (4.229) we have modeled an incompressible fluid.

Besides this material equation for an incompressible fluid we have to solve the Navier-Stokes equation

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = -\partial_k p + \eta^{\mathrm{s}} \Delta v_k + f_k. \tag{4.230}$$

Here ϱ is the mass density, f_k the external force per unit volume, p denotes the pressure field, and η^{s} is the shear viscosity. The first term vanishes because we look for a stationary solution. The second term $v_i \partial_i v_k$ vanishes as well with Eq. (4.229). There are no external forces, $f_k = 0$. The pressure gradient must be constant, we denote it by $\partial_3 p = -\Delta p / L$. L is the tube length and Δp the pressure difference between entry and exit.

The equation to be solved is

$$\eta^{\mathrm{s}} \left\{ f'' + \frac{f'}{r} \right\} = -\frac{\Delta p}{L}. \tag{4.231}$$

The prime stands for the derivative with respect to r. The solution which is regular at $r = 0$ and vanishes at $r = R$ is given by

$$v_3 = f(r) = \frac{\Delta p}{4\eta^{\mathrm{s}} L}(R^2 - r^2). \tag{4.232}$$

4.11.2 Flux

The flux[28] passing through the tube is

$$\dot{V} = 2\pi \int_0^R \mathrm{d}r\, r\, v_3 = \frac{\pi}{8\eta^{\mathrm{s}}} R^4 \frac{\Delta p}{L}. \tag{4.233}$$

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[28] Measured in $\mathrm{m}^3\,\mathrm{s}^{-1}$.

This law—the flux is proportional to the fourth power of the inner tube radius—was discovered independently by the German engineer Gotthilf Hagen and the French physician Jean Louis Poiseuille. The former was responsible for the water supply of Berlin, the latter studied the flow of blood.

The Hagen-Poiseuille law is only valid for a laminar flow where one layer glides smoothly over the next layer. See the article on *Reynolds' Number* for the transition from laminar to turbulent flow.

Let us work out the power required to pump the volume $\dot{V}$ per unit time through a tube. There are at least three approaches to this problem.

4.11.3 Pump Power

(a) The mean velocity $\bar{v}$ is

$$\bar{v} = \frac{1}{\pi R^2} \int_0^R \mathrm{d}r\, 2\pi r\, v_3(r) = \frac{\Delta p}{8\eta^{\mathrm{s}} L} R^2. \tag{4.234}$$

$\Delta p\, \pi R^2$ is the net force exercised on the cross section, and if multiplied by the average velocity, we calculate

$$P = \dot{V}\, \Delta p. \tag{4.235}$$

A plausible result. First, its physical dimension is energy per time. Second, the more liquid we want to pump through a tube, the more power we need to do so. If the tube is small, more pressure difference is required to pump the same amount of liquid, and the pumping effort grows correspondingly.

(b) But why do we have to use energy for pumping the liquid? Right, there is internal friction, and mechanical energy is transferred into heat. While flowing, the liquid gets warmer, and the tube radiates off this internal energy. According to Eq. (1.93) the production of internal energy by friction[29] is described by

$$\pi(U) = T''_{jk} G_{jk}, \tag{4.236}$$

where T''_{jk} is the irreversible contribution to the stress tensor and G_{jk} denotes the symmetric velocity gradient. The latter is

$$G_{13} = G_{31} = \frac{\Delta p}{4\eta^{\mathrm{s}} L} x_1 \text{ and } G_{23} = G_{32} = \frac{\Delta p}{4\eta^{\mathrm{s}} L} x_2, \tag{4.237}$$

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[29] Velocity gradients.

the remaining entries vanish. According to Eq. (2.11) we may write

$$T''_{jk} = 2\eta^{\mathrm{s}} G_{jk}. \tag{4.238}$$

The volumetric production rate of internal energy is

$$\pi(U) = \frac{(\Delta p)^2}{2\eta^{\mathrm{s}} L^2} r^2, \tag{4.239}$$

and the integral over the interior of the entire pipe can be shown to be equal to $\dot{V}\Delta p$, the same as Eq. (4.235).

(c) One can also work out the shear force on the interior wall of the pipe. It points in z-direction and is given by

$$F_3 = \int_0^L \mathrm{d}z \int_0^{2\pi} \mathrm{d}\phi\, R\, \left(T''_{31}\frac{x_1}{R} + T''_{32}\frac{x_2}{R}\right) = \Delta p\, \pi R^2. \tag{4.240}$$

A not so plausible result: the force is the product of the pressure difference, ok, and the cross section. One would have expected the circumference.

If this force is multiplied by the average speed $\bar{v}$ of Eq. (4.234) we obtain $\dot{V}\Delta p$ as well. The idea is that the liquid is at rest and we move the pipe with velocity $\bar{v}$.

4.12 Ice Layer

In this example we shall study the growing or melting of an ice layer, a typical Stefan problem. It is not only internal energy which has to be transported from cooler to warmer regions. In addition, there is a heat source from freezing or a heat sink from melting. From a mathematical point of view, we have two differential equations to solve simultaneously. One is the heat equation within the ice layer, the other one concerns the location of the solid to liquid phase transition.

4.12.1 Phase Transition Enthalpy

Consider one mole of water at atmospheric pressure p_{at}. Its temperature T depends on the internal energy U within the system. If we increase U by heating, the temperature will increase as well. However, if the system is in its solid phase (ice), and if the temperature has reached the melting point $T_{\mathrm{m}} = 0\,°\mathrm{C}$, the temperature will remain constant. Added heat is used to melt more and more of the ice, until the system is entirely in its liquid phase, or water in the narrower sense. The amount of heat to melt one mole of water at constant atmospheric pressure is traditionally called the *latent melting heat* or *heat of fusion*.

However, the term *fusion enthalpy* is more appropriate. Enthalpy, a thermodynamic potential, is defined by $H = H(S, p) = U + pV$ where S, p, U, V denote entropy, pressure, internal energy and volume, respectively. Its partial derivatives are given by

$$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}p. \tag{4.241}$$

For reversible processes, $T\mathrm{d}S$ may be identified with $\mathrm{d}Q$, the amount of internal energy transferred by heat, not work. Consequently, heating a probe at constant pressure increases its enthalpy. The specific[30] fusion enthalpy of water at atmospheric pressure $p = p_{\mathrm{at}}$ is $\Delta H_{\mathrm{sl}} = 3.34 \times 10^5\,\mathrm{J\,kg^{-1}}$. The suffix sl denotes the solid to liquid phase transition.

4.12.2 The Problem

Denote by x the depth below a lake's surface. There is an ice layer of thickness $s = s(t)$ which changes in the course of time. Within the ice layer the heat transport equation

$$\dot{T} = \kappa T'' \tag{4.242}$$

has to be solved for the temperature field $T = T(t, x)$. The constant κ, also called the temperature conductivity, is an abbreviation for

$$\kappa = \frac{\lambda}{\varrho C_{\mathrm{p}}}. \tag{4.243}$$

λ denotes the heat conduction coefficient as defined in Fourier's law,

$$\boldsymbol{J}^{\mathrm{u}} = -\lambda \nabla T. \tag{4.244}$$

The current density of internal energy, or the heat current density, is proportional to the temperature gradient, from warm to cold. ϱ is the mass density of ice, and C_{p} denotes the specific heat of ice at constant pressure. The heat equation (4.242) has to be solved for $0 < x < s(t)$. Recall that the thickness $s = s(t)$ of the ice layer will depend on time.

We simplify the problem by assuming $T(t, 0) = T_0$ and $T(t, x) = T_{\mathrm{m}}$ for $x \le s(t)$. The surface temperature shall be constant, the temperature at the bottom of the ice layer and below is the melting temperature of 0°C. This is not completely

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[30] In this context: per unit mass.

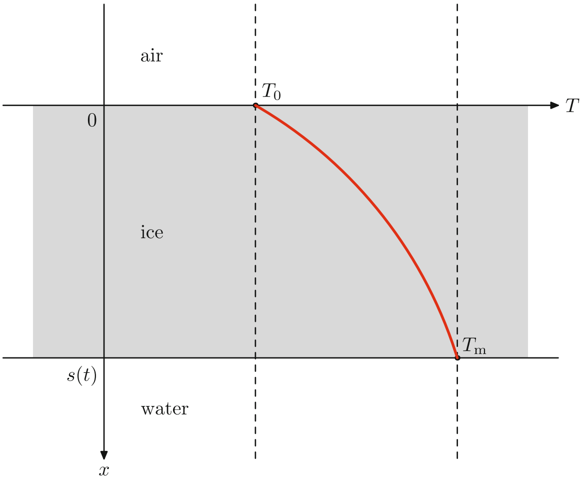

Fig. 4.9 Depth vs. temperature of an ice layer. The model assumes a constant temperature T_0 at the air/ice interface and the melting temperature T_m of 0°C at and below the ice/water interface. The temperature $T = T(t, x)$ within the ice layer and the thickness $s = s(t)$ of it are the subject of this article

realistic since very deep lakes have a temperature of 4°C at the bottom. See Fig. 4.9 for a sketch.

Consider an area $\mathrm{d}A$ at the interface between ice and water. During the short time $\mathrm{d}t$ the layer will grow by $\mathrm{d}x = \dot{s}(t)\,\mathrm{d}t$. The volume $\mathrm{d}V = \dot{s}(t)\mathrm{d}t\,\mathrm{d}A$ has been undergone the liquid-solid phase transition thereby liberating the amount $\mathrm{d}Q = \varrho\,\mathrm{d}V\,\Delta H$ of heat. This heat must be transported by conduction, $\mathrm{d}Q = -\mathrm{d}A\,\mathrm{d}t J^\mathrm{u} = \mathrm{d}A\,\mathrm{d}t\,\lambda\,T'(t, s(t))$. The temperature gradient refers to the ice/water interface. Lumping all this together leads to the following ordinary differential equation:

$$\dot{s}(t) = \alpha\,T'(t, s(t)) \text{ with } \alpha = \frac{\lambda}{\varrho\,\Delta H} = \frac{C_\mathrm{p}\,\kappa}{\Delta H}. \tag{4.245}$$

Note that thermal conductivity, mass density or specific heat capacity refer to ice.

Let us summarize the problem. The heat equation (4.242) for the temperature field $T = T(t, x)$ is to be solved for $t \geq 0$ and $0 \leq x \leq s(t)$. The temperature boundary values are $T(t, 0) = T_0$ and $T(t, s(t)) = T_\mathrm{m}$, i.e., for a free boundary. The free boundary itself obeys Eq. (4.245). Both differential equations are intimately coupled, since the solution of the heat equation depends on the boundary, and the boundary equation requires the temperature gradient at the free boundary.

4.12.3 Crude Approximation

If heat conduction is assumed to be a fast process as compared with melting or freezing, one might argue as follows. Assume that the temperature changes linearly with depth,

$$T(t,x) \approx T_0 + \frac{T_\mathrm{m} - T_0}{s(t)} x. \tag{4.246}$$

Then the temperature gradient at the ice/water interface is

$$T'(t, s(t)) \approx \frac{T_\mathrm{m} - T_0}{s(t)}, \tag{4.247}$$

and Eq. (4.245) reads

$$\dot{s} \approx \alpha \frac{T_\mathrm{m} - T_0}{s}. \tag{4.248}$$

This differential equation may be solved by the separation of variables method, the result, with $s(0) = 0$, is

$$s(t) = \sqrt{2\alpha\,(T_\mathrm{m} - T_0)\,t}. \tag{4.249}$$

This crude approximation will be compared with the analytical solution which we shall derive later. It should be the solution for small Stefan numbers S. Read on.

4.12.4 Dimensionless Quantities

Let us first convert the Stefan problem at hand into a form with dimensionless quantities. We introduce a reference length ℓ such that $\xi = x/\ell$ is the dimensionless length. Likewise a dimensionless temperature $\theta = (T - T_0)/(T_\mathrm{m} - T_0)$ will be used. The heat equation becomes

$$\frac{\partial\theta}{\partial\tau} = \frac{\partial^2\theta}{\partial\xi^2} \tag{4.250}$$

if a dimensionless time $\tau = t\,\kappa/\ell^2$ is introduced. We look for a temperature field $\theta = \theta(\tau, \xi)$. With $s = \sigma\ell$ one writes

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\tau} = S\,\frac{\partial\theta}{\partial\xi}\bigg|_{\xi=\sigma(\tau)}. \tag{4.251}$$

The dimensionless Stefan constant is

$$S = \frac{C_\mathrm{p}\,(T_m - T_0)}{\Delta H}. \tag{4.252}$$

By the way, C_p for ice is $2.1 \times 10^3\,\mathrm{J\,kg^{-1}\,K^{-1}}$. For a temperature difference $T_0 - T_\mathrm{m}$ of 10°C and with $\Delta H = 3.34 \times 10^5\,\mathrm{J\,kg^{-1}}$, the problem is characterized by a Stefan constant of $S = 0.063$.

We look for a field $\theta = \theta(\tau, \xi)$ and a function $\sigma = \sigma(\tau)$ which satisfy the differential equations (4.250) and (4.251). These functions have to obey the boundary conditions

$$\theta(\tau, 0) = 0 \text{ and } \theta(\tau, \sigma(\tau)) = 1 \tag{4.253}$$

as well as

$$\sigma(0) = 0. \tag{4.254}$$

Fumbling with ℓ cannot make the Stefan constant S to be unity by retaining a value one for the temperature conductivity. In fact, from a physical point of view, there is no inherent unit of length, and therefore we are confronted with differential equations and boundary conditions which do not contain ℓ, the reference length. And: just because of this there is an analytical solution.

4.12.5 The Exact Solution

Guided by the crude approximation (4.249) we introduce the variable $z = \xi/2\sqrt{\tau}$ and try the following *ansatz*:

$$\theta(\tau, \xi) = f(z). \tag{4.255}$$

The heat equation (4.250) says

$$f'' + 2zf' = 0 \text{ or } g' + 2zg = 0 \text{ with } g(z) = f'(z). \tag{4.256}$$

Its solution with $\theta(\tau, 0) = 0$, or $f(0) = 0$ is

$$f(z) = a \int_0^z \mathrm{d}\zeta \; \mathrm{e}^{-\zeta^2}. \tag{4.257}$$

Now, try $\sigma(\tau) = b\sqrt{\tau}$, in accordance with Eq. (4.249). One obtains

$$\frac{\mathrm{d}\sigma(\tau)}{\mathrm{d}\tau} = \frac{b}{2\sqrt{\tau}} = S\frac{\partial\theta(\tau, \sigma(\tau))}{\partial\xi} = Sa\,\mathrm{e}^{-b^2/4}\,\frac{1}{2\sqrt{\tau}}, \tag{4.258}$$

or

$$b = Sa\,\mathrm{e}^{-b^2/4}. \tag{4.259}$$

The remaining boundary condition to be met is

$$\theta(\tau, \sigma(\tau)) = a \int_0^{b/2} \mathrm{d}\zeta \; \mathrm{e}^{-\zeta^2} = 1. \tag{4.260}$$

We eliminate a and arrive at the following transcendental equation

$$b\,\mathrm{e}^{b^2/4}\int_0^{b/2}\mathrm{d}\zeta\;\mathrm{e}^{-\zeta^2} = S \tag{4.261}$$

for the yet unknown constant b in $\sigma(\tau) = b\sqrt{\tau}$. The left hand side behaves as $b^2/4$ for small b and increases monotonically to infinity with $b \to \infty$. Hence, Eq. (4.261) has a unique solution for any Stefan number S. Once b is known, the constant a in Eq. (4.257) can be determined from Eq. (4.259).

By the way, our crude approximation presented above is nothing else but the exact solution for a small Stefan number, i.e., $b = 2\sqrt{S}$. If this number is small, heat production at the ice/water interface is so slow that the temperature increases linearly from T_0 to T_{m} which would be the solution of the heat equation for a constant boundary at $x = s$. Note that, for small b, the temperature is linear in z, hence linear in x for each time t.

4.12.6 Discussion

In this article we have presented a model for freezing or melting of ice. In order to provide an analytical solution we have over-simplified the situation. We have assumed that the interface between air and ice, a lake's surface, is at a constant temperature. Daily or yearly variations should be considered. Moreover, the water beneath the ice layer was assumed to be at the melting temperature for ice, or the freezing temperature of water. However, water at large depths has a temperature of 4°C which corresponds to the maximal mass density. Hence heat conduction between the ice/water interface and deeper regions must be taken into account. Also the air/ice interface must be described more accurately.

Stefan was confronted with measurements of the ice cap thickness around the north pole. Now his name is connected with a class of differential equations where parts of the boundary are not fixed, but determined by the solution. There is a rich literature on numerical procedures all of which are tested on the exact solution which we have presented here.

4.13 Metamaterials

Metamaterials are artificial regular structures, one, two, or three-dimensional, which provide for exceptional interactions with electromagnetic waves. Always within a certain frequency interval, practically any desired permittivity and permeability can be mimicked, such as a negative permittivity, a negative permeability, or both values negative.

Metamaterials are first of all materials, and not devices. They appear to be homogeneous. Their interaction with electromagnetic waves is described by complex-valued (relative) permittivities ϵ_{ij} and permeabilities μ_{ij}. Metamaterials are meta, or transcending the category of materials, because they are modified by structures, or circuits, on a micrometer or nanometer scale. Metamaterials[31] may exhibit properties not found in natural materials.

Modifications on a micrometer scale are relatively easy to fabricate, they affect the interaction with microwaves. Ever better methods of nanometer scale manipulations and self-replication techniques will soon allow for exciting applications in optics. The field of metamaterials is rather new and still dominated by theoretical investigations, but advances in nanoskills promise a bright future of this interdisciplinary effort.

A recent monograph on "Waves in Metamaterials" by Solymar and Shamonina [12] is warmly recommended for detailed studies.

Photonic crystals are another type of artificial materials for advanced optical applications. The permittivity of a photonic crystal varies regularly with a spatial frequency comparable with that of light. This results in optical band gaps: frequency ranges where light cannot propagate.

4.13.1 Resonances

A standard metamaterial is made up of a regular array of identical resonators the spacing of which is small as compared with the wavelength of harmonically oscillating traveling electromagnetic fields, that is microwaves or light waves.

Natural optical materials are arrays of copies of the crystallographic unit cell, each acting as an antenna. They are excited by an incoming oscillating electric field and, with a certain phase shift, emit an outgoing oscillating electric field. The fields are superimposed and averaged. Magnetic fields play no role. This explains why natural optical materials are characterized by a magnetic permeability $\mu = 1$.

In contrast, the resonators of a metamaterial are usually LC circuits. They affect the electric and the magnetic field. Consequently, after averaging, the dielectric permittivity $\epsilon = \epsilon(\omega)$ and the magnetic permeability $\mu = \mu(\omega)$ are affected.

Now, resonators are weakly coupled damped harmonic oscillators responding with large signals if excited close to certain eigen- or resonance frequencies. The same applies to spatially averaged resonator properties, that is, to permittivity ϵ and permeability μ. Close to such a resonance frequency, the material may exhibit both a negative permittivity *and* a negative permeability.

The best studied resonator (for microwave metamaterials) is a pair of split rings, one inside the other. We show just one example which has been investigated experimentally by Gundogdu et al. [2] and many others (Fig. 4.10).

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[31] The word seems to be reserved for microwave and optical applications.

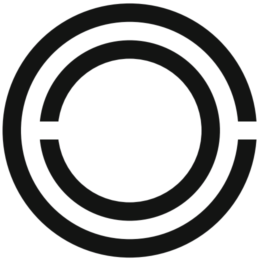

Fig. 4.10 A split ring resonator. When excited by an electromagnetic wave, charge in the rings flows in opposite direction giving rise to a magnetic field. Likewise, charges of different sign produce an electric field in the splits and between the rings. This LC resonator supports resonating waves which are much longer than the dimension of the outer ring

4.13.2 Wave Propagation

Maxwell's equations, if applied to plane waves

$$\tilde{F}\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,, \tag{4.262}$$

in absence of free charges and currents read

$$\boldsymbol{k}\times\tilde{\boldsymbol{H}} = -\omega\epsilon\epsilon_0\tilde{\boldsymbol{E}} \text{ and } \boldsymbol{k}\times\tilde{\boldsymbol{E}} = \omega\mu\mu_0\tilde{\boldsymbol{H}}, \tag{4.263}$$

in usual notation. The remaining divergence equations are satisfied automatically.

Note that a real field $F = F(t,\boldsymbol{x})$ can be written in terms of its Fourier transform as

$$\begin{aligned} F(t,\boldsymbol{x}) &= \int\frac{\mathrm{d}\omega}{2\pi}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\,\tilde{F}(\omega,\boldsymbol{k})\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \\ &= \int_0^\infty\frac{\mathrm{d}\omega}{2\pi}\int\frac{\mathrm{d}^3k}{(2\pi)^3}\tilde{F}(\omega,\boldsymbol{k})\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} + \text{c.c.} \end{aligned} \tag{4.264}$$

The Fourier transform now extends over positive frequencies only, but has to be augmented by the complex conjugate expression. In the following we always assume frequencies to be positive or zero, but we omit the c.c. hint.

Let us write $\boldsymbol{k} = k\hat{\boldsymbol{k}}$ where the unit vector $\hat{\boldsymbol{k}}$ defines the direction of wave propagation. The polarization vector $\hat{\boldsymbol{e}}$ is orthogonal to it. With $\tilde{\boldsymbol{E}} = \tilde{E}\hat{\boldsymbol{e}}$ one obtains

$$\tilde{\boldsymbol{H}} = \frac{k\tilde{E}}{\omega\mu\mu_0}\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}}. \tag{4.265}$$

Inserting this into Eq. (4.263) yields the dispersion relation

$$k^2 = \epsilon\mu\,\frac{\omega^2}{c^2} \text{ or } k = nk_0, \tag{4.266}$$

with $c = \sqrt{1/\epsilon_0\mu_0}$ as the speed of light in empty space. We abbreviated ω/c by k_0, the vacuum wave number of the monochromatic light source under study. According to our convention on frequencies, this number is never negative.

$$n = \sqrt{\epsilon\mu} \tag{4.267}$$

is the refractive index. Generally, the electric and the magnetic field strength of light waves are related by

$$\tilde{\boldsymbol{H}} = \frac{n\tilde{E}}{c\mu_0\mu}\hat{\boldsymbol{k}}\times\hat{\boldsymbol{e}}. \tag{4.268}$$

The Poynting vector $\boldsymbol{S} = \boldsymbol{E}\times\boldsymbol{H}$ of a plain wave thus has four contributions. $\tilde{\boldsymbol{E}}^*\times\tilde{\boldsymbol{H}}^*$ and $\tilde{\boldsymbol{E}}\times\tilde{\boldsymbol{H}}$ oscillate with angular frequencies 2ω and -2ω, respectively. They do not contribute to field energy transport. The remainder does not oscillate, it is

$$\boldsymbol{S} = 2\,\mathrm{Re}\,\tilde{\boldsymbol{E}}\times\tilde{\boldsymbol{H}}^*. \tag{4.269}$$

We calculate

$$\boldsymbol{S} = \frac{2n}{c\mu_0\mu}|\tilde{E}|^2\,\hat{\boldsymbol{k}}. \tag{4.270}$$

Natural materials are characterized by $\mu = 1$ and $\epsilon(\omega) > 0$. Then the refractive index (4.267) is positive and, according to Eq. (4.269), energy and the wave propagate in the same direction. We therefore speak of a *forward* material. In contrast, metamaterials, in a certain frequency range, may be characterized by negative values of both permittivity and permeability. In this case, the refractive index is still positive, but Eq. (4.269) says that energy and the wave propagate in opposite direction. A medium with this property is called a *backward* material.

4.13.3 Normal Refraction

We will now recapitulate the normal situation: a beam passes the interface between two different natural materials. We index the medium at $y > 0$ by I and $y < 0$ by II. Figure 4.11 sketches the situation. Note that we have plotted the wave vectors $\boldsymbol{k}^{\mathrm{i}}$, $\boldsymbol{k}^{\mathrm{r}}$ and $\boldsymbol{k}^{\mathrm{t}}$ of an incident, reflected and transmitted beam, respectively.

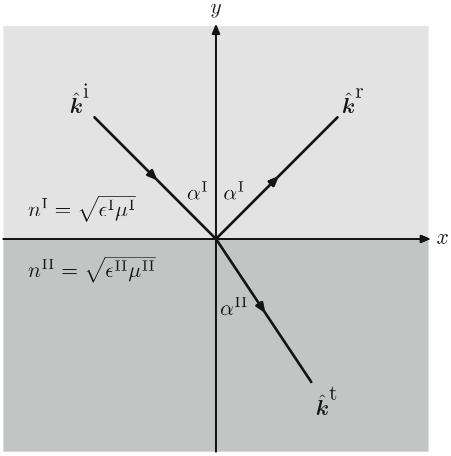

Fig. 4.11 An incident light wave which propagates in direction $\hat{\boldsymbol{k}}^{\mathrm{i}}$ is partly reflected ($\hat{\boldsymbol{k}}^{\mathrm{r}}$) and transmitted ($\hat{\boldsymbol{k}}^{\mathrm{t}}$) at the interface $y = 0$ between two different optical media

In order to be specific, we consider perpendicularly polarized light, perpendicular with respect to the x, y-plane of incidence. It is well known that at least three waves are required to solve the problem. We try

$$\begin{aligned}\tilde{\boldsymbol{E}}^{\mathrm{i}} &= E^{\mathrm{i}}\hat{e}_z\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{I}}(\sin\alpha^{\mathrm{i}}x - \cos\alpha^{\mathrm{i}}y)}\,,\\ \tilde{\boldsymbol{E}}^{\mathrm{r}} &= E^{\mathrm{r}}\hat{e}_z\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{I}}(\sin\alpha^{\mathrm{r}}x + \cos\alpha^{\mathrm{r}}y)}\,,\\ \tilde{\boldsymbol{E}}^{\mathrm{t}} &= E^{\mathrm{t}}\hat{e}_z\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{II}}(\sin\alpha^{\mathrm{t}}x - \cos\alpha^{\mathrm{t}}y)}\,.\end{aligned} \tag{4.271}$$

At the interface $y = 0$ the tangential component of the electric field must be continuous, at all x and at all times t. The latter condition has already been taken into account: the angular frequencies of all three waves are the same. $\tilde{\boldsymbol{E}}_x$ vanishes and is therefore continuous. $\tilde{\boldsymbol{E}}_z(x, 0, z)$ is continuous if

$$E^{\mathrm{i}} + E^{\mathrm{r}} = E^{\mathrm{t}} \tag{4.272}$$

as well as

$$n^{\mathrm{I}}\sin\alpha^{\mathrm{i}} = n^{\mathrm{I}}\sin\alpha^{\mathrm{r}} = n^{\mathrm{II}}\sin\alpha^{\mathrm{t}} \tag{4.273}$$

hold true. Note that the electric field is given by $\tilde{\boldsymbol{E}}^{\mathrm{i}} + \tilde{\boldsymbol{E}}^{\mathrm{r}}$ in the upper and by $\tilde{\boldsymbol{E}}^{\mathrm{t}}$ in the lower half-space.

Equation (4.273) says that the angle of incidence $\alpha^{\mathrm{i}} = \alpha^{\mathrm{I}}$ and of reflexion $\alpha^{\mathrm{r}} = \alpha^{\mathrm{I}}$ are the same. Moreover, Snell's law of refraction must hold for $\alpha^{\mathrm{t}} = \alpha^{\mathrm{II}}$, namely

$$n^{\mathrm{I}}\sin\alpha^{\mathrm{I}} = n^{\mathrm{II}}\sin\alpha^{\mathrm{II}}. \tag{4.274}$$

At the interface, the normal component $\epsilon\tilde{\boldsymbol{E}}_y$ vanishes and is therefore continuous.

Let us now study the continuity properties of the magnetic field. It is made up of these three waves:

$$\begin{aligned}
\tilde{\boldsymbol{H}}^{\mathrm{i}} &= \frac{n^{\mathrm{I}} E^{\mathrm{i}}}{c\mu_0\mu^{\mathrm{I}}}(-\cos\alpha^{\mathrm{I}}\hat{\boldsymbol{x}} - \sin\alpha^{\mathrm{I}}\hat{\boldsymbol{y}})\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{I}}(\sin\alpha^{\mathrm{I}}x - \cos\alpha^{\mathrm{I}}y)}\,,\\
\tilde{\boldsymbol{H}}^{\mathrm{r}} &= \frac{n^{\mathrm{I}} E^{\mathrm{r}}}{c\mu_0\mu^{\mathrm{I}}}(\cos\alpha^{\mathrm{I}}\hat{\boldsymbol{x}} - \sin\alpha^{\mathrm{I}}\hat{\boldsymbol{y}})\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{I}}(\sin\alpha^{\mathrm{I}}x + \cos\alpha^{\mathrm{I}}y)}\,,\\
\tilde{\boldsymbol{H}}^{\mathrm{t}} &= \frac{n^{\mathrm{II}} E^{\mathrm{t}}}{c\mu_0\mu^{\mathrm{II}}}(-\cos\alpha^{\mathrm{II}}\hat{\boldsymbol{x}} - \sin\alpha^{\mathrm{II}}\hat{\boldsymbol{y}})\,\mathrm{e}^{\mathrm{i}k_0 n^{\mathrm{II}}(\sin\alpha^{\mathrm{II}}x - \cos\alpha^{\mathrm{II}}y)}\,.
\end{aligned} \tag{4.275}$$

The components $\tilde{\boldsymbol{H}}_x$, $\tilde{\boldsymbol{H}}_z$ and $\mu\tilde{\boldsymbol{H}}_y$ must be continuous at $y = 0$.

For $\tilde{\boldsymbol{H}}_x$ this implies [14]

$$\frac{n^{\mathrm{I}}\cos\alpha^{\mathrm{I}}}{\mu^{\mathrm{I}}}(E^{\mathrm{i}} - E^{\mathrm{r}}) = \frac{n^{\mathrm{II}}\cos\alpha^{\mathrm{II}}}{\mu^{\mathrm{II}}}E^{\mathrm{t}} \tag{4.276}$$

and Eq. (4.273). $\tilde{\boldsymbol{H}}_z$ vanishes and is therefore continuous. That $\mu\tilde{\boldsymbol{H}}_y$ shall be continuous is the same as Eqs. (4.272) and (4.273). Equations (4.273) and (4.276) allow to work out the energy current densities (power) carried by the three waves.

4.13.4 Refraction in a Backward Medium

Let us now study the above problem if one half space is a backward medium. In order to simplify the discussion we assume that $y > 0$ is an ideal backward medium, characterized by $\epsilon^{\mathrm{I}} = \mu^{\mathrm{I}} = -1$, while $y < 0$ is an ideal forward medium, namely the vacuum with $\epsilon = \mu = +1$. None of the equations above have to be modified, we just have to specialize them.

The refractive indexes of both media are $n^{\mathrm{I}} = n^{\mathrm{II}} = 1$. Equation (4.273) says that all angles are equal. Equation (4.272) remains unchanged, $E^{\mathrm{i}} + E^{\mathrm{r}} = E^{\mathrm{t}}$. However, Eq. (4.275) becomes $E^{\mathrm{r}} - E^{\mathrm{i}} = E^{\mathrm{t}}$. Together, these two continuity requirements result in $E^{\mathrm{i}} = 0$ and $E^{\mathrm{t}} = E^{\mathrm{r}}$. Moreover, Eq. (4.270) says that the formerly reflected beam is now incident while the formerly incident beam has vanished. We sketch this in Fig 4.12.

Although we have demonstrated the strange refraction behavior for perpendicular polarization, the same holds true for parallel polarization. Hence, even an unpolarized beam will be bent as depicted in Fig. 4.12. And the same is true if the beam passes from vacuum to an ideal backward medium: the normal component of the Poynting vector is continuous, the transversal component changes sign.

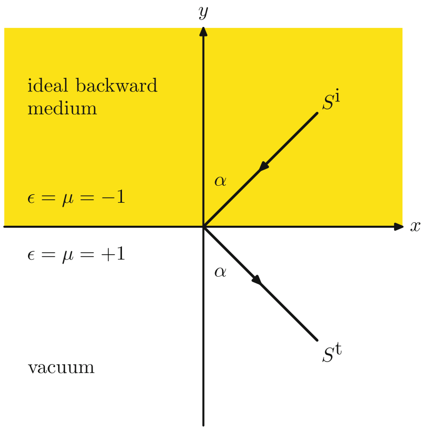

Fig. 4.12 The power flow of a beam which passes from an ideal backward material (*upper half*) to an ideal forward medium (vacuum). The *arrows* represent Poynting vectors, not unit wave vectors as in Fig. 4.11. The formerly incident beam is absent, the formerly reflected beam is now incident

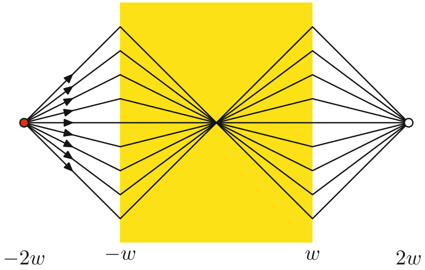

Fig. 4.13 A parallel slab of ideal backward material. It maps the upward object at the *left* into an equally large upward image at the *right*. Here we demonstrate the imaging of a point source (*filled dot*)

4.13.5 A New Type of Optical Microscope

Among the many interesting applications of this effect we mention just one. A parallel plate of ideal backward material may serve as a lens, as depicted in Fig. 4.13. Denote the plate width by $2w$. The plane at the distance w to the left is mapped into a plane at distance w to the right. Upward pointing objects are mapped into upward pointing objects.

Imaging by a backward medium allows to transfer the information in the near field. Conventional optical microscopes employ the information of the far field only, they are limited by diffraction. Metamaterials allow to transcend this limit.

4.13.6 Photonic Crystals

A photonic crystal is a material the optical permittivity of which varies in a regular pattern. Since the propagation of light is concerned, they are called photonic. They are called crystals because the permittivity modulations are regular, albeit the lattice constant is in the micrometer range, not nanometers. Photonic crystals can be arrays of regularly spaced identical rib waveguides (1D), arrays of boreholes (2D), or regularly staples of 2D photonic crystals. A photonic crystal in the narrower sense is a material with an optical band gap. A plane wave with wave vector $\boldsymbol{k}$ travels with an angular frequency $\omega = \omega(\boldsymbol{k})$. For a photonic crystal there is an interval of frequency values for which there is no wave vector. Waves of these forbidden frequencies cannot propagate in a photonic crystal giving rise to remarkable applications.

In order to demonstrate the phenomenon of an optical band gap we work out an extremely simple model. We consider a regular staple of two kind of slabs. The unit cell is the region $-a/2 \leq x \leq a/2$. There is a slab of higher refractive index n_2 for $-d/2 \leq x \leq d/2$, and outside it the refractive index is n_1. This unit cell is copied and translated by the lattice constant a, N times say.

We consider a plane wave traveling along x. With

$$\boldsymbol{E}(t, \boldsymbol{x}) = \begin{pmatrix} 0 \\ E(x) \\ 0 \end{pmatrix} \mathrm{e}^{-\mathrm{i}\omega t} \tag{4.277}$$

we have to solve

$$E''(x) + k_0^2 \epsilon(x) E(x) = 0 \text{ where } k_0 = \frac{\omega}{c}. \tag{4.278}$$

The permittivity $\epsilon(x)$ has the value n_2^2 in the high index slab and n_1^2 outside it.

In each region of constant permittivity the solution is of the form

$$E(x) = a_+ \mathrm{e}^{+\mathrm{i}k_0 n x} + a_- \mathrm{e}^{-\mathrm{i}k_0 n x}, \tag{4.279}$$

where a_+ is the amplitude of the plane wave traveling in x-direction while a_- denotes the amplitude of the wave propagating in counter-direction. These amplitudes at different positions x depend linearly upon each other to be described by 2 × 2 transfer matrices.

The propagation in a region of constant refractive index n by a distance y is described by

$$P(n, y) = \begin{pmatrix} \mathrm{e}^{+\mathrm{i}k_0 n y} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}k_0 n y} \end{pmatrix}. \tag{4.280}$$

At a position where the refractive index jumps from n' on the left to n'' to the right, continuity requirements are to be observed. In our case, the functions

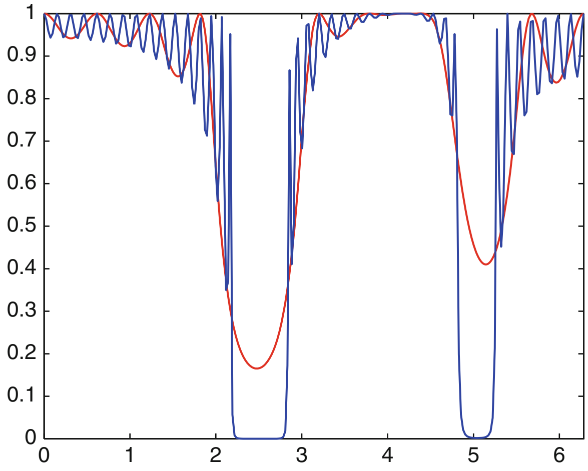

Fig. 4.14 Transmission coefficient versus $k_0 a = \omega a/c$. The smoother curve corresponds to 4 unit cells, the curve with more variations to 16 unit cells. There are frequency regions where the structure does not transmit waves

$E = E(x)$ and $E' = E'(x)$ must be continuous, the latter being proportional to the 3-component of the magnetic field strength. It is a simple task to show that the transfer matrix

$$D(n', n'') = \frac{1}{2n''} \begin{pmatrix} n'' + n' & n'' - n' \\ n'' - n' & n'' + n' \end{pmatrix} \tag{4.281}$$

fulfills the continuity requirements. Note that D is the unity matrix if there is no discontinuity.

The passage of light through one unit cell is therefore described by the transfer matrix

$$T = P\left(n_1, \frac{a-d}{2}\right) D(n_1, n_2) P(n_2, d) D(n_2, n_1) P\left(n_1, \frac{a-d}{2}\right). \tag{4.282}$$

The transfer matrix of N adjacent unit cells is $T_N = T^N$.

We work out

$$T_N \begin{pmatrix} 0 \\ a_t \end{pmatrix} = \begin{pmatrix} a_r \\ a_i \end{pmatrix}. \tag{4.283}$$

There is an incident wave impinging on the right with amplitude a_i running from right to left. The reflected wave has the amplitude a_r. a_t is the amplitude of the transmitted wave. The transmittance coefficient is defined by

$$t = \frac{|a_t|^2}{|a_i|^2}. \tag{4.284}$$

We have plotted it in Fig. 4.14 for a structure of four and sixteen unit cells. The refractive indexes are $n_1 = 1.0$ (air) and $n_2 = 1.5$ (glass). The ratio $d/a = 0.5$ means that slabs of air and glass are equally thick.

Already for only 16 unit cells, the frequency band gaps are clearly visible. Note that the transfer matrix T is unitary which guarantees that the sum of transmitted and reflected intensity equals the incident intensity. For frequencies in the band gap the photonic crystal is an ideal reflector.

This is not the right place to go into details of manufacturing and applications of photonic crystals. Although such crystals are not continuous media proper, they form a new class of interesting materials which can be tailored to a large extent. Reference [11] is a valuable source of detailed information.

4.14 Model Atmosphere

In this brief article we study a remarkably accurate model of the earth's atmosphere, at least for the lower part of its troposphere. The troposphere is the 15 km thin layer which is governed by weather phenomena. There is an hourly change of temperature and pressure, there are clouds, up- and down as well as lateral motion of air masses, and so forth. To set up all relevant balance- and material equations, to digitize the problem and to feed in observational data and calculate a reliable weather forecast is a formidable job. In fact, only with powerful supercomputers a sufficiently accurate prediction can be made which is faster than the actual progress of time. This is not the main focus of this book.

Instead, we derive a material equation for air which describes rapid mixing due to hourly temperature changes. If an air bubble suddenly moves upwards, its volume will immediately adjusts to the new environment, but there is no time for energy exchange by heat conduction: the process is adiabatic. Either the bubble is too heavy with respect to its new environment, and it will sink, or it is too light, and it will rise even further. One speaks of convection instability. We assume that rising or sinking air bubbles are in equilibrium with their environment, i.e., that the atmosphere is labile with respect to adiabatic convection.

4.14.1 Adiabatic Process for a Diatomic Ideal Gas

Denote by $F = F(T, V)$ the free energy of n moles of a fluid medium of homogeneous composition. T denotes temperature, and V is the volume. Entropy S and pressure p are partial derivatives,

$$\mathrm{d}F = -S\mathrm{d}T - p\mathrm{d}V. \tag{4.285}$$

We integrate this for an ideal gas,

$$p = \frac{nRT}{V}, \tag{4.286}$$

of diatomic molecules,

$$C_V = T\frac{\partial S}{\partial T} = \frac{5}{2}nR. \tag{4.287}$$

$R = 8.314\ \mathrm{J\,K^{-1}\,mol^{-1}}$ is the universal gas constant, and C_V denotes the heat capacity at constant volume. Equation (4.287) says that there are three translational and two rotational degrees of freedom, each contributing with $k_B T/2$ per molecule. Vibrational degrees of freedom are frozen, and interactions are supposed to be negligible.

Equations (4.286) and (4.287) may be integrated and yield

$$F(T,V) = F_0 - S_0(T-T_0) - \frac{5}{2}nRT\ln\frac{T}{T_0} - nRT\ln\frac{V}{V_0}, \tag{4.288}$$

where T_0 and V_0 refer to a reference state with $F_0 = F(T_0, V_0)$ and $S_0 = S(T_0, V_0)$.

Lines of constant entropy are characterized by

$$S_0 + \frac{5}{2}nR\ln\frac{T}{T_0} + nR\ln\frac{V}{V_0} = \text{const.} \tag{4.289}$$

The system in two states (T_1, V_1) and (T_2, V_2) has the same entropy if

$$\frac{T_1}{T_2}\left\{\frac{V_1}{V_2}\right\}^{2/5} = 1 \tag{4.290}$$

holds true. An equivalent formulation is

$$\frac{T_1}{T_2} = \left\{\frac{p_1}{p_2}\right\}^{2/7}. \tag{4.291}$$

4.14.2 Convection Neutral Atmosphere

The atmosphere's temperature $T = T(z)$ and pressure $p = p(z)$ depend on the height z above ground level. Within the troposphere temperature and pressure change hourly, and air bubbles sink or rise steadily. If a bubble rises from z to $z + \mathrm{d}z$, its temperature changes according to

$$\tau = T(x)\left\{\frac{p(z+\mathrm{d}z)}{p(z)}\right\}^{2/7}. \tag{4.292}$$

If the air bubble temperature τ is larger than $T(z + \mathrm{d}z)$, the bubble is too hot as compared with the environment, and it will rise further. Likewise, if τ is smaller than $T(z + \mathrm{d}z)$, it will sink. In both cases there will be up- or downward transport of air mass until equilibrium is attained. This equilibrium is characterized by $\tau = T(z + \mathrm{d}z)$, or

$$\frac{T'}{T} = \frac{2}{7}\frac{p'}{p}, \tag{4.293}$$

where the prime denotes differentiation with respect to z.

The atmosphere as described by $T = T(z)$ and $p = p(z)$ is neutral to the ascend or descend of air masses if Eq. (4.293) is fulfilled. There are still lateral movements of air masses (winds) because the condition for a convection neutral atmosphere depends on the situation at ground level.

From a technical point of view Eq. (4.293) is a material equation, just as the ideal gas law (4.286). It describes the relation between temperature and pressure of a diatomic ideal gas if there is no heat energy transport. Material equations not only characterize the material under study, they also take details of processes into account.

Let us now concentrate on the solution. First of all, the equation of hydrostatic equilibrium has to be fulfilled, namely

$$p' = -g\varrho, \tag{4.294}$$

where $p = p(z)$ denotes the pressure and $\varrho = \varrho(z)$ the mass density. The symbol $g = 9.81\ \mathrm{m\,s^{-2}}$ stands for the gravitational acceleration close to the earth's surface. We arrive at

$$\frac{-p'}{p} = \frac{g\varrho_0 T_0}{p_0}\frac{1}{T} = -\frac{7}{2}\frac{T'}{T}. \tag{4.295}$$

This implies that the temperature decreases linearly with height,

$$T(z) = T_0\left\{1 - \frac{z}{H}\right\}, \tag{4.296}$$

where

$$H = \frac{7}{2}\frac{p_0}{g\varrho_0} \approx 30\ \mathrm{km}. \tag{4.297}$$

Air pressure decreases according to

$$p(z) = p_0\left\{1 - \frac{z}{H}\right\}^{7/2}. \tag{4.298}$$

H roughly defines the troposphere, the weather region. Formally, at $z = H$, the atmospheric pressure and temperature would become zero. In fact, the model of neutral adiabatic convection breaks down already at a height of 10 to 18 km, depending on latitude. Normally, a temperature of −57°C indicates tropopause, the height at which weather does no more influence the state of the atmosphere.

Discussing the state of the earth's atmosphere turns out to be rather complicated. What is the zero height level? What is temperature in the presence of the sun's radiation? How to measure air pressure close to an airplane which necessarily modifies its surrounding, and so forth. Meteorology has become a scientific discipline in its own right, however firmly based on the laws of continuum physics.

4.15 Natural Units

In this book on *Continuum Physics* we study continuously distributed ordinary matter. Ordinary matter is a neutral collection of nuclei and electrons at low temperatures. The electrons move slowly as compared with the speed of light such that the prevailing force is governed by Coulomb's law, and all this within the framework of quantum theory. Consequently, the mass m of the electron, its charge $-e$, $4\pi\epsilon_0$ and Planck's constant $\hbar$ will enter the stage if properties of ordinary matter are discussed. Even *White Dwarfs* are made up of ordinary matter in this sense.

This book adheres strictly to the SI system of units.[32] The unit of mass is the kilogram (kg). Lengths are measured in meters (m) and time in seconds (s). The fourth base unit is the ampere (A) for an electric current.

4.15.1 SI and Atomic Units

The above mentioned constants of nature are

- $\hbar = 1.054572 \times 10^{-34}\,\mathrm{kg\,m^2\,s^{-1}}$
- $e = 1.602177 \times 10^{-19}\,\mathrm{s\,A}$
- $m = 9.109383 \times 10^{-31}\,\mathrm{kg}$
- $4\pi\epsilon_0 = 1.112650 \times 10^{-10}\,\mathrm{kg^{-1}\,m^{-3}\,s^4\,A^2}$

Their dimensions are summarized in Table 4.1.

The matrix of powers in Table 4.1 can be inverted. It gives rise to Table 4.2 which describes how a physical SI-unit can be expressed as a product of powers of the involved constants of nature.

The atomic energy unit, also called Hartree, is given by

$$E^* = \frac{me^4}{(4\pi\epsilon_0)^2\hbar^2} = 27.2\,\mathrm{eV}. \tag{4.299}$$

The natural unit of length is

$$a^* = \frac{4\pi\epsilon_0\hbar^2}{me^2}, \tag{4.300}$$

---

[32] *Système international d'unités* in French.

Table 4.1 Physical dimension of the four constants of nature which govern the physics of ordinary matter. The numbers indicate the power of the corresponding SI unit

	kg	m	s	A
$\hbar$	1	2	−1	0
e	0	0	1	1
m	1	0	0	0
$4\pi\epsilon_0$	−1	−3	4	2

Table 4.2 SI-units expressed as products of powers of constants of nature

	$\hbar$	e	m	$4\pi\epsilon_0$
kg	0	0	1	0
m	2	−2	−1	1
s	3	−4	−1	2
A	−3	5	1	−2

which evaluates to 0.529 Å = 52.9 pm. The natural unit of length a^* is also known as Bohr's radius.

The natural unit of time is

$$\tau^* = \frac{\hbar^3(4\pi\epsilon_0)^2}{me^4} = 2.49 \times 10^{-17}\,\text{s}, \tag{4.301}$$

the corresponding angular frequency is

$$\omega^* = \frac{2\pi}{\tau^*} = 2.60 \times 10^{17}\,\text{Hz}. \tag{4.302}$$

In order to decide whether an electric field is small one has to compare with

$$\mathcal{E}^* = \frac{m^2e^5}{(4\pi\epsilon_0)^3\hbar^4} = 0.514 \times 10^{12}\,\text{Vm}^{-1}. \tag{4.303}$$

Likewise, a magnetic induction has to be compared with

$$\mathcal{B}^* = \frac{e^3m^2}{\hbar^3(4\pi\epsilon_0)^2} = 2.35 \times 10^5\,\text{T}. \tag{4.304}$$

T (tesla) is the SI-unit of magnetic induction, the same as $\text{V}\,\text{s}\,\text{m}^{-2}$.

The following short `MATLAB` program allows to calculate the atomic unit for any physical dimension:

```
function [value,power]=atomic_unit(si)
val=[1.05457e-34,1.60218e-19,9.10938e-31,4*pi*8.85419E-12];
dim=[1 2 -1 0; 0 0 1 1; 1 0 0 0; -1 -3 4 2];
```

```
mid=round(inv(dim));
power=si*mid;
value=prod(val.^power);
```

`si` is a vector of the powers of kg, m, s, and A (SI units of mass, length, time and electric current). The result is the value of the corresponding atomic unit and the powers of $\hbar$, e, m, and $4\pi\epsilon_0$, respectively.

Bohr's radius, for example, is calculated as

```
>> length=[0 1 0 0];
>> [astar,powers]=atomic_unit(length);
```

It returns

`astar=5.2917...e-11`

and

`powers=[2 -2 -1 1].`

Compare this with Eq. (4.300).

4.15.2 Remarks

The Schrödinger equation for the hydrogen atom becomes

$$\left\{ -\frac{1}{2}\Delta - \frac{1}{r} \right\} \psi = E\psi, \tag{4.305}$$

in natural units. Its solutions are $E = -1/2n^2$ for $n = 1, 2, \ldots$. Hence the ground state energy of the hydrogen atom is $-1/2$ atomic units, or $-13.6\,\text{eV}$. This and more complicated equations reduce to the essentials if formulated in atomic units. The ground state energy of the hydrogen atom is a typical example. Its value is a number close to 1 multiplied by its natural size which depends on the system of units. The latter value is easy to work out, all the effort of theoretical physics is to calculate the number in front of it, here $-1/2$.

Another example are elasticity moduli. They have the physical dimension of pressure, or energy density. The atomic unit of pressure is

$$p^* = \frac{E^*}{{a^*}^3} = \frac{m^4 e^{10}}{\hbar^8 (4\pi\epsilon_0)^5} = 29.42\,\text{TPa}. \tag{4.306}$$

Compare this with $E \approx 200\,\text{GPa}$ for Young's elasticity module for steel. Although the order of magnitude is all right, the ratio $E/p^* \approx 0.01$ is rather small. But bear in mind that a few powers of 4π may soon lead to large or small numbers. Moreover, the size of an atom depend on the charge of its nucleus, and so forth. And we might have compared E with eV/Å^3. Work it out! See the article on the *Pockels and Kerr Effect* for another example.

A final remark concerns the speed of light. c, the vacuum light speed, is another constant of nature. Atomic physics is inherently non-relativistic. Relativistic effects have to be introduced as corrections. The natural unit of speed is

$$v^{*}=\frac{m^{2}}{\hbar 4\pi\epsilon_{0}}=2.1877\times 10^{6}\,\mathrm{m\,s^{-1}}. \tag{4.307}$$

The ratio

$$\alpha=\frac{v^{*}}{c}=\frac{m^{2}}{\hbar c 4\pi\epsilon_{0}}\approx\frac{1}{137} \tag{4.308}$$

is called the fine structure constant. It is a dimensionless number, less than 1%.

Have a look at the defining equation for the electromagnetic field:

$$\dot{\boldsymbol{p}}=q\{\boldsymbol{E}+\boldsymbol{v}\times\boldsymbol{B}\}. \tag{4.309}$$

This definition, although very convenient from an engineer's point of view, is nevertheless unsatisfactory: the electric field and its magnetic counterpart have different physical dimensions. From

$$\dot{\boldsymbol{p}}=q\left\{\boldsymbol{E}+\frac{\boldsymbol{v}}{c}\times c\boldsymbol{B}\right\} \tag{4.310}$$

one concludes that both fields, $\boldsymbol{E}$ and $c\boldsymbol{B}$, are directly comparable. The natural counterpart of the electric field strength is the induction field strength multiplied by the velocity of light.

4.16 Ohm's Law and Hall Effect

Without an external electric field, the electric current normally vanishes in thermal equilibrium. Superconductivity is a particular case which we will not address here. An external electric field polarizes matter, and the polarization grows linearly with the electric field strength, over many orders of magnitude. If the electric field varies with time, so does the polarization. Its time derivative is nothing else but the electric conduction current which then is proportional to the electric field strength (Ohm's law). The proportionality factor is the electric conductivity which depends on the angular frequency ω of the electric field. We speak of an electrical conductor if the conductivity does not vanish with $\omega\to 0$.

In the following we describe the classical Drude model for conductivity. In general, the conductivity is a second rank tensor, and we discuss the consequences of time reversal invariance (Onsager relations). We also investigate the dependency of the conductivity on an external quasi-static induction field (Hall effect). And finally, we argue why the electric field strength should be replaced by the negative gradient of the electrochemical potential since it is irrelevant whether the charge current is driven by the gradient of an electric potential or by the electron's chemical potential.

4.16.1 Drude Model

The classical Drude model has been mentioned in this book elsewhere, in the articles on the *Faraday Effect* as well as on *Surface Optical Waveguide*. In the former case it served to qualitatively explain the influence of a quasi-static induction on the dielectric permittivity of optically transparent media. We also could explain the complex permittivity of noble metals for sufficiently large wavelengths. Here we focus on the conductivity of an electrical conductor in the presence of an external quasi-static induction.

A typical quasi-free electron has mass m, charge $-e$ and a friction constant $m\Gamma$. We assume the electric field $E = E(t)$ to point along the 1-direction and an induction $\mathcal{B}$ along the 2-direction. The location $\boldsymbol{x} = \boldsymbol{x}(t)$ of the electron obeys the following equation of motion:

$$m\begin{pmatrix}\ddot{x}_1\\ \ddot{x}_2\\ \ddot{x}_3\end{pmatrix} + m\Gamma\begin{pmatrix}\dot{x}_1\\ \dot{x}_2\\ \dot{x}_3\end{pmatrix} = -eE(t)\begin{pmatrix}1\\0\\0\end{pmatrix} - e\mathcal{B}\begin{pmatrix}-\dot{x}_3\\ 0\\ \dot{x}_1\end{pmatrix}. \tag{4.311}$$

$x_2(t) = 0$ is an obvious solution. Fourier transforming Eq. (4.311) gives

$$m\omega\{-\omega - \mathrm{i}\Gamma\}\begin{pmatrix}\tilde{x}_1\\ 0\\ \tilde{x}_3\end{pmatrix} = -e\tilde{E}(\omega)\begin{pmatrix}1\\0\\0\end{pmatrix} + \mathrm{i}\omega e\mathcal{B}\begin{pmatrix}-\tilde{x}_3\\ 0\\ \tilde{x}_1\end{pmatrix}. \tag{4.312}$$

Let us assume $\mathcal{B} = 0$ for a moment. The solution of Eq. (4.312) then is

$$\tilde{x}_1 = \frac{e}{m\omega(\omega + \mathrm{i}\Gamma)}\,\tilde{E}\;,\; \tilde{x}_2 = 0 \text{ and } \tilde{x}_3 = 0. \tag{4.313}$$

For small $\mathcal{B}$ (in natural units) we insert the above into Eq. (4.312) and obtain

$$\tilde{x}_3 = -\mathrm{i}\frac{e}{m^2\omega(\omega + \mathrm{i}\Gamma)^2}\,\mathcal{B}\,\tilde{E}. \tag{4.314}$$

$-e\tilde{\boldsymbol{x}}$ is the dipole moment of one electron, of which there are N per unit volume. The polarization therefore is $-eN\tilde{\boldsymbol{x}}$, its time derivative

$$\tilde{\boldsymbol{J}}^{\mathrm{e}}(\omega) = -\mathrm{i}\omega N(-e)\tilde{\boldsymbol{x}}(\omega) = \frac{Ne^2}{m(\Gamma - \mathrm{i}\omega)}\,\tilde{\boldsymbol{E}}, \tag{4.315}$$

in the absence of an external induction. We conclude that the conductivity σ is given by

$$\tilde{\boldsymbol{J}}^{\mathrm{e}}(\omega) = \sigma(\omega)\,\tilde{\boldsymbol{E}}(\omega) \text{ with } \sigma(\omega) = \frac{Ne^2}{m(\Gamma - \mathrm{i}\omega)}. \tag{4.316}$$

The first equation is Ohm's law: the electric current density is proportional to the electric field, both oscillating with the same angular frequency ω. The proportionality factor $\sigma = \sigma(\omega)$ likewise depends on ω. Its DC[33] value $\sigma(0)$ is finite and positive, irrespective of the sign of e. It does not matter whether electrons or holes transport charge. For high frequencies the conductivity becomes complex which describes the retardation between applied field and resulting current density.

If there is an external induction field, the electric current acquires an addition which is proportional to the electric field and the induction and perpendicular to both. This phenomenon is known as Hall effect. We do not bother to write down the expression for $\tilde{J}_3$ corresponding to Eq. (4.314). Later we argue why we should introduce an electric field $\tilde{E}_3$ which make $\tilde{J}_3$ vanish.

4.16.2 Onsager Relations

In Chap. 3 we derived explicit expressions for permittivities and conductivities. Although difficult or impossible to work them out, they allow to establish rules which are independent on the special system under study. They are valid for an arbitrary Hamiltonian which specifies the system under study. Onsager's relations for conductivities are of this type.

In general, the relationship between the driving electric field $\tilde{E}_j$ and the electric current density $\tilde{J}_i^{\mathrm{e}}$ is linear:

$$\tilde{J}_i^{\mathrm{e}}(\omega) = \sigma_{ij}(\omega)\,\tilde{E}_j(\omega), \tag{4.317}$$

the conductivity is described by a tensor.

This tensor does not only depend on angular frequency ω, but also on all the external parameters which affect the thermodynamic equilibrium, like temperature T, strain S, external static electric field $\boldsymbol{\mathcal{E}}$ or magnetic induction $\boldsymbol{\mathcal{B}}$, and so forth. Onsager's relations in our case state

$$\sigma_{ij}(\omega; T, S, \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}) = \sigma_{ji}(\omega; T, S, \boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}). \tag{4.318}$$

Transposing the conductivity tensor *and* inverting the magnetic induction is a symmetry.

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[33] DC means direct current, as contrasted with AC, alternating current.

4.16.3 Hall Effect

Let us keep temperature and strain constant. The external static electric field has already been taken into account since $\boldsymbol{\mathcal{E}} = \tilde{\boldsymbol{E}}(0)$. For the dependency on the induction we write

$$\sigma_{ij}(\omega; \boldsymbol{\mathcal{B}}) = \sigma_{ij}(\omega) + H_{ijk}(\omega)\mathcal{B}_k + \cdots, \tag{4.319}$$

where the dots indicate terms which are of higher order in the induction. Onsager's relations demand the H_{ijk} be antisymmetric in the first pair of indexes, the answer to which is the Levi-Civita symbol,

$$H_{ijk}(\omega) = \epsilon_{ijk} H(\omega). \tag{4.320}$$

Equation (4.320) says

$$\tilde{J}_i^{\mathrm{e}}(\omega) = \sigma_{ij}(\omega)\tilde{E}_j(\omega) + H(\omega)\epsilon_{ijk}\tilde{E}_j(\omega)\mathcal{B}_k. \tag{4.321}$$

The first contribution describes Ohm's law, the conductivity being a symmetric tensor. The second term causes the Hall effect.

Normally, the boundary conditions forbid a current perpendicular to $\tilde{\boldsymbol{E}}$ and $\boldsymbol{\mathcal{B}}$. Then, charges are displaced such that an electric counter-field builds up which stops the Hall current. Assume an electrically isotropic medium where the driving electric field E_x is applied along the 1-direction and the induction $\mathcal{B}_y$ along the 2-direction, as assumed above. The current flows in 1-direction, its density is $J_x = \sigma E_x$. The Hall current $HE_x\mathcal{B}_y$ would flow in 3-direction, but it cannot, because a field E_z stops it, such that $\sigma E_z + HE_x B_y = 0$ holds true. One may reformulate this as

$$E_z = -\frac{HE_x\mathcal{B}_y}{\sigma} = -\frac{HJ_x\mathcal{B}_y}{\sigma^2} = R_{\mathrm{H}} J_x \mathcal{B}_y, \tag{4.322}$$

where $R_{\mathrm{H}} = -H/\sigma^2$ is the frequency dependent Hall constant. Kaye and Laby [5] cite $R_{\mathrm{H}} = 0.75\ \mathrm{V\,m\,A^{-1}\,T^{-1}}$ for indium arsenide, a semiconductor with interesting properties.

By the way, the Hall constant can be interpreted as $R_{\mathrm{H}} = -1/Nq$ where N is the density of charge carriers and q their charge. This is the result of the above Drude model calculation. Its sign therefore lets decide whether electrons or holes are responsible for charge transport. The size of the Hall constant is a good measure for the carrier density. Note, however, that the simple interpretation of the Hall constant is valid only if there is just one kind of charge carriers.

Unfortunately, discussing the quantum Hall effect is out of the scope of this small book on *Continuum Physics*.

4.16.4 Electro-Chemical Potential

So far we have argued that it is the electric field strength $\boldsymbol{E} = -\nabla\phi^{\mathrm{e}}$ which causes quasi-free electrons to move. The electric field drags mobile electrons, and because there are interactions of all types, which amount to friction, there is a steady stream of charge. The stronger the dragging force, the larger the charge current density. This is Ohm's law in a nutshell.

However, mobile electrons may also migrate because their chemical potential changes from place to place. This effect, electron diffusion, will also cause a charge current density. In fact, the two causes for the movement of electrons are inseparable. We have discussed this in the section on *Charge Transport*.

Denote by μ^* the chemical potential of electrons and by ϕ^{e} the electric potential. The electrochemical potential is defined as

$$\psi = \phi^{\mathrm{e}} - \frac{\mu^*}{e}. \tag{4.323}$$

Both contributions drive electrons likewise, and therefore Ohm's law should be reformulated as

$$J^{\mathrm{e}} = -\sigma_{ij}\,\partial_j\,\psi. \tag{4.324}$$

Differences $\Delta\psi$ of the chemical potential are sometimes called *electromotive forces* (emf).

The electrochemical potential is a key notion in electrochemistry. Chemical reactions in batteries, fuel cells and so forth serve to drive electric currents. A wide field which, again, we cannot cover here.

4.17 Optically Active Media

There are screw-like media which rotate the polarization vector of linearly polarized light. In contrast to the Faraday effect, where the left- or right handedness is brought about by a magnetic field, optically active media are reciprocal. If the beam travels through the medium in backward direction, the rotation of the polarization vector is undone. Quartz and suspensions of natural grape sugar are well known examples.

For light of sufficiently low intensity the relationship between electric field strength and induced polarization is described by the susceptibility tensor,

$$\tilde{P}_i(\omega, \boldsymbol{k}) = \chi_{ij}(\omega, \boldsymbol{k})\tilde{E}_j(\omega, \boldsymbol{k}). \tag{4.325}$$

We have explained this in detail in Chap. 3 and briefly in our articles on *Crystal Optics*, the *Pockels* and *Kerr Effect* and the *Faraday Effect*. In all these cases it was sufficient to evaluate the susceptibility at $\boldsymbol{k} = 0$. Here we shall investigate the dependency on the wave vector in more detail.

Phonons

A solid medium, ideally, is either a dielectric, an electric conductor or something in-between, a semi-conductor. The valance electrons of a crystal are grouped in bands. If all bands are filled, we speak of a dielectric. If the uppermost[34] band is half-filled, we speak of a conductor. If the material is a dielectric, but the energy gap between the completely filled band and the next one is rather small, we speak of a semiconductor. With increasing temperature, more and more electrons can jump from the lower almost filled energy band to the higher almost empty energy band. There are mobile electrons in the almost empty energy band and missing electrons, or holes, in the almost full energy band below. If electrons or electron holes are mobile, light will be absorbed strongly by inducing transitions. For a dielectric this is impossible since the energy gap between the full band and the above empty band is too large. Therefore, the typical material required for optical applications is a dielectric like lithium niobate, yttrium iron garnet, quartz, water or glass. All these materials have in common that their electric conductivity vanishes. The interaction between light is not with mobile electrons, but with phonons, the quanta of elastic vibrations.

Phonons have an energy $\hbar\omega$, a momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$, and are polarized, either longitudinally (L) or transversely (T1 and T2). The dispersion relation $\omega = \omega_\alpha(\boldsymbol{k})$ for α = L, T1 and T2, can be calculated or measured by neutron refraction. If the unit cell of the crystal contains more than one ion, there are acoustical and optical branches. The former are of the form $\omega_\alpha^{\text{ac}}(\boldsymbol{k}) = c_\alpha|\boldsymbol{k}| + \cdots$, where c_α is the speed of sound for longitudinal or transverse sound waves. The acoustical phonon dispersion curves will never intersect the photon[35] dispersion curve $\omega(\boldsymbol{k}) = c|\boldsymbol{k}|$. However, the optical phonon branches vary like $\omega_\alpha^{\text{op}}(\boldsymbol{k}) = \omega_\alpha^{\text{op}}(0) - \omega_\alpha'' k^2/2 + \cdots$, they will always intersect the photon dispersion curve. However, measured in natural units,[36] k will be very small.

This section is intended to elucidate a possible dependency of the susceptibility $\chi(\omega, \boldsymbol{k})$ on the wave number $\boldsymbol{k}$. The mechanism which we have discussed here is just one of many more, it pertains to polaritons which are important for infrared light. In general, the susceptibility depends on the wave vector $\boldsymbol{k}$ because the interaction of electromagnetic waves and matter is non-local.

4.17.1 *Spatial Dispersion*

The angular frequency ω and the wave vector $\boldsymbol{k}$ in Eq. (4.325) are not independent. After all, the electromagnetic field has to obey Maxwell's equations which, for this purpose, read

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[34] With respect to energy.

[35] c is the vacuum speed of light.

[36] See the article on *Natural Units*.

$$(k^2\delta_{ij} - k_i k_j)\,\tilde{E}_j = \left(\frac{\omega}{c}\right)^2 (\delta_{ij} + \chi_{ij})\,\tilde{E}_j. \tag{4.326}$$

We write

$$\boldsymbol{k} = n\,\frac{\omega}{c}\,\hat{\boldsymbol{n}} \text{ and } \tilde{\boldsymbol{E}} = E\,\hat{\boldsymbol{e}}, \tag{4.327}$$

where n is the refractive index, $\hat{\boldsymbol{n}}$ the propagation direction, a unit vector, and $\hat{\boldsymbol{e}}$ denotes the polarization, likewise a unit vector. With these symbols the wave equation (4.326) becomes

$$n^2(\delta_{ij} - \hat{n}_i\hat{n}_j)\,\hat{e}_j = (\delta_{ij} + \chi_{ij})\,\hat{e}_j. \tag{4.328}$$

There are two cases to be distinguished:

- Longitudinal polarization: $\hat{\boldsymbol{n}} \parallel \hat{\boldsymbol{e}}$. Equation (4.328) has no solution. Equation (4.326) leads to $\omega = 0$. The electromagnetic field is static.
- Transversal polarization: $\hat{\boldsymbol{n}} \perp \hat{\boldsymbol{e}} = 0$. n^2 is an eigenvalue of the permittivity tensor $\epsilon_{ij} = \delta_{ij} + \chi_{ij}$ and $\hat{\boldsymbol{e}}$ the corresponding eigenvector.

However, there is a flaw in the above chain of arguments: the dependency of $\chi_{ij}(\omega, \boldsymbol{k})$ on $\boldsymbol{k}$ has been ignored. Equation (4.328) implies the following procedure. Specify an angular frequency ω and a polarization $\hat{\boldsymbol{e}}$. Work out $\chi_{ij} = \chi_{ij}(\omega, 0)$. Then solve Eq. (4.328) for n^2 and $\hat{\boldsymbol{n}}$. One solution will be $\hat{\boldsymbol{n}} = \hat{\boldsymbol{e}}$, discard it. The remaining two solutions provide refractive indexes n and propagation directions $\hat{\boldsymbol{n}}$ of plane light waves. Put otherwise, we assumed $\boldsymbol{k} = 0$ and have worked out the propagation vector $\boldsymbol{k}$. This article tries to remedy this inconsistency, at least in linear approximation. The propagation constants for light will not only depend on the angular frequency ω, but also on the wave vector $\boldsymbol{k}$. The former effect is called dispersion, but it should be called temporal dispersion. The latter effect therefore is spatial dispersion.

4.17.2 Optical Activity

The interaction between light and a dielectric medium is strongest if phonons and photons are in resonance, that is, they have the same energy and momentum. We have argued above that this happens for small wave vectors only, in natural units. Therefore we postulate a linear dependency of the susceptibility tensor on the wave vector:

$$\chi_{ij}(\omega, \boldsymbol{k}) = \chi_{ij}(\omega) + \chi^{\text{oa}}_{ijk}(\omega) k_k + \cdots. \tag{4.329}$$

As demonstrated in Chap. 3, time reversal invariance requires the Onsager relation

$$\chi_{ij}(\omega, \boldsymbol{k}; \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}) = \chi_{ji}(\omega, -\boldsymbol{k}; \boldsymbol{\mathcal{E}}, -\boldsymbol{\mathcal{B}}). \tag{4.330}$$

We have exploited this

- For $\boldsymbol{k} = \boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{B}} = 0$ in the article on *Crystal Optics*,
- For $\boldsymbol{k} = \boldsymbol{\mathcal{B}} = 0$ in the article on the *Pockels* and *Kerr Effect*,
- For $\boldsymbol{k} = \boldsymbol{\mathcal{E}} = 0$ in the article on the *Faraday Effect*,

and we shall now discuss the situation $\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{B}} = 0$ but $\boldsymbol{k} \neq 0$.

The susceptibility tensor (4.329), which should also be Hermitian, can be written as

$$\chi_{ij}(\omega, \boldsymbol{k}) = \chi_{ij}(\omega) + \mathrm{i}\epsilon_{ijk} g_k(\omega) \text{ with } g_k(\omega) = G_{kl}(\omega) k_l. \tag{4.331}$$

Since the Levi-Civita symbol ϵ_{ijk} is a pseudo-tensor of rank three, the so-called gyration vector g_k must be a pseudo-vector and G_{kl} a pseudo-tensor of rank two.

G_{kl} cannot be measured directly because it has to be contracted with the wave vector $\boldsymbol{k}$ which characterizes the solution. It is an object of theoretical study, only certain crystal symmetries allow for it. Here it suffices to demonstrate that the gyration vector $\boldsymbol{g}$ is a pseudo-vector which changes sign if $\boldsymbol{k}$ is inverted. The latter feature distinguishes it from the gyration vector which describes the Faraday effect. Equation (4.202) may be rewritten as Eq. (4.331) with

$$g_k = K \mathcal{B}_k, \tag{4.332}$$

where $\boldsymbol{\mathcal{B}}$ is the quasi-static external magnetic induction. This gyration vector does not change sign if the propagation vector $\boldsymbol{k}$ of a wave is inverted.

Consider a linearly polarized wave which travels along the direction $\hat{\boldsymbol{g}}$ of the gyration vector

$$\boldsymbol{g} = g \hat{\boldsymbol{g}} \tag{4.333}$$

of an optically active medium. If it travels a distance ℓ, the polarization vector will be rotated by an amount $\Phi^{\mathrm{oa}} \ell$. The specific[37] rotation is

$$\Phi^{\mathrm{oa}} = \frac{g k_0}{2n} = \pi \frac{g}{n \lambda_0}. \tag{4.334}$$

n is the refractive index, k_0 and λ_0 denote the vacuum wave number and wavelength of light, respectively. Equation (4.334) is a symbol-by-symbol translation of the corresponding formula (4.211) for the specific Faraday rotation.

4.17.3 Quartz

Chemically, quartz is silicon dioxide, SiO_2. Its crystal form at room temperature, also called α-quartz, lacks an inversion plane. Optically, it is a transparent uniaxial

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[37] In this context: per unit length.

mineral with an ordinary index of refraction of 1.5442 and an extraordinary of 1.5533. The optical axis $\hat{\boldsymbol{c}}$, however, is a pseudo-vector. Quartz may be either left handed or right handed. Single large crystals are either totally left handed or totally right handed, and sometimes twins with left handed and right handed domains. Statistically, there is no preference for handedness. The laws of nature do not seem to prefer right handedness to left handedness.

The effects of birefringence are usually much larger than optical activity. Only for the ordinary beam, which travels along the optical axis $\hat{\boldsymbol{c}}$, the rotation of the polarization vector can be observed. For quartz at room temperature and for $\lambda = 0.633\,\mu\text{m}$ the specific rotation is $18.7°\,\text{mm}^{-1}$, according to Kaye and Laby [5].

The properties of a light beam are judged by an observer who looks into the beam.[38] Right handed quartz rotates the polarization vector counter-clockwise. Let the thumb of a right hand point into the propagation direction of a beam. The fingers then indicate the sense of polarization rotation.

Light propagating not in, but counter to the optical axis of a right-handed quartz will also be right handed. Therefore, a right handed quartz, if rotated by 180° around an axis which is perpendicular to the optical axis, will also be right-handed.

4.17.4 Natural Grape Sugar

Glucose is a simple sugar, or monosaccharide. Its summary formula is $C_6H_{12}O_6$. It is produced by the green plants out of water and carbon dioxide and energy, thereby releasing oxygen. It is burnt, finally, with oxygen, to water and carbon dioxide providing energy. The glucose molecule comes in two species, one being the mirror of the other. There are D-glucose molecules[39] the structure of which resembles a right-handed screw. The mirror molecule is named L-glucose, it resembles a left-handed screw. Both forms have the same binding energy and should be equally probable. Indeed, this is the case if glucose is synthesized artificially. Naturally produced glucose, however, is always of the D-type, or dextrose. It is produced in wine grapes and therefore also known as grape sugar. It is also known as blood sugar because all other nutrients like starch and similar carbon hydrates, fats and proteins are transformed by the human digestive systems into D-glucose which may enter cells and power them.

Physically speaking, a D-glucose molecule is characterized by a unit axial vector $\hat{\boldsymbol{c}}$ describing its orientation as right-handed. In a solution, for instance in water, the $\hat{\boldsymbol{c}}$ vectors of the D-glucose molecules are randomly distributed. The average, however will not result in zero because $\hat{\boldsymbol{c}}$ and $-\hat{\boldsymbol{c}}$ affect light equally.

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[38] What you should not do!

[39] Latin *dexter*, right handed.

A solution of D-glucose is optically isotropic. Any direction will serve as optical axis. Its optical activity is proportional to the concentration. This provides a convenient method for determining the D-glucose concentration in blood. Normal values are 100 mg per dL (100 cm^3), or 1.00 g per liter blood. Since a normal grown-up person has approximately 6 L of blood, already 6 g of grape sugar will double the natural concentration practically immediately. Other sugars, like cane sugar, milk sugar and so forth are broken down to D-glucose by the digestive system, they increase the blood sugar level as well, but with a certain retardation.

4.18 Pockels and Kerr Effect

The propagation of light in a transparent medium is governed by the susceptibility tensor. It describes the polarization response of the medium, in linear approximation, to perturbations by a rapidly oscillating electric field. The response is retarded, therefore the susceptibility depends on the light wavelength, or angular frequency. Moreover, the susceptibility is an expectation value, it depends on all parameters which describe the thermodynamic equilibrium of the medium under study. Each of these gives rise to a branch of optics:

- Temperature: thermo-optics
- Stress: photo-elasticity, acousto-optics
- Quasi-static electric field: electrooptics
- Quasi-static magnetic field: magnetooptics

Here we study electrooptic effects. The susceptibility tensor depends on the quasi-static electric field strength $\mathcal{E}$. We call it quasi-static, because it is an equilibrium parameter. However, even if it changes with time in the gigahertz (GHz) range, the thermodynamic equilibrium can follow instantaneously. This has to be compared with the frequency of light which is one million times larger (PHz). At these frequencies, which correspond to photon energies of electron volts (eV), matter reacts with a noticeable retardation. One speaks of the Pockels effect if the crystal's symmetry allows for a suitable rank three tensor, such that susceptibility changes linearly with the external electric field. If there is no Pockels effect, the quadratic Kerr effect, although much smaller, allows to manipulate the propagation of light. Modern integrated optical devices rely on dielectric waveguides with micrometer dimensions: high electric field strengths can be achieved by rather small voltages.[40] Integrated optics has become an engineering science which we cannot even be touched upon in this small book with its emphasis on balance and material equations.

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[40] Ten volts per micrometer correspond to hundred thousand Volts per centimeter.

4.18.1 Dielectric Susceptibility

We assume a linear and causal relationship between the light wave's electric field strength and the polarization caused by it,

$$P_i(t,\boldsymbol{x}) = \int_0^\infty \mathrm{d}\tau \int \mathrm{d}^3\xi \; \Gamma_{ij}(\tau,\boldsymbol{\xi})\, E_j(t-\tau,\boldsymbol{x}-\boldsymbol{\xi}). \tag{4.335}$$

Any field $f = f(t,\boldsymbol{x})$ may be decomposed uniquely in harmonious contributions:

$$f(t,\boldsymbol{x}) = \int \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t} \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\; \tilde{f}(\omega,\boldsymbol{k}), \tag{4.336}$$

such that Eq. (4.335) becomes

$$\tilde{P}_i(\omega,\boldsymbol{k}) = \epsilon_0 \chi_{jk}(\omega,\boldsymbol{k})\, \tilde{E}_j(\omega,\boldsymbol{k}). \tag{4.337}$$

As long as the response (polarization) depends linearly on the perturbation (light electric field strength), both oscillate with the same temporal and spatial frequencies $(\omega,\boldsymbol{k})$ multiplied by the susceptibility $\chi_{ij}(\omega,\boldsymbol{k})$. Susceptibility χ_{ij} and response function Γ_{ij} of Eq. (4.335) are related by

$$\chi_{ij}(\omega,\boldsymbol{k}) = \frac{1}{\epsilon_0}\int_0^\infty \mathrm{d}\tau\; \mathrm{e}^{\mathrm{i}\tau\omega} \int \mathrm{d}^3\boldsymbol{\xi}\; \mathrm{e}^{-\mathrm{i}\boldsymbol{\xi}\cdot\boldsymbol{k}}\; \Gamma_{ij}(\tau,\boldsymbol{\xi}). \tag{4.338}$$

In general, the dependency on the wave vector $\boldsymbol{k}$ is so weak that we may neglect it.[41]

In the chapter on *Linear Resonse Theory*, we derived an explicit expression for the response functions Γ_{ij} as an equilibrium expectation value of a certain commutator. This expression allowed to prove a number of properties:

- Refraction and absorption: the susceptibility tensor $\chi_{ij} = \chi'_{ij} + \mathrm{i}\,\chi''_{ij}$ can be split into a Hermitian and an anti-Hermitian part. The former describes refraction, the latter absorption of light.
- Kramers-Kronig relation: the Hermitian part $\chi'_{ij}(\omega)$ at a certain frequency ω is a particular integral of the anti-Hermitian part $\chi''_{ij}(u)$ at different frequencies u. No refraction without absorption, albeit at possibly far away frequencies.
- Onsager relation: the susceptibility is invariant with respect to interchanging its indexes, provided an external induction field $\mathcal{B}$ is reversed as well, $\chi_{ij}(\mathcal{B}) = \chi_{ji}(-\mathcal{B})$.

If there is no quasi-static external induction field, but an electric field $\mathcal{E}$, the susceptibility tensor is symmetric.

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[41] *Optical activity* is an exception.

4.18.2 Pockels Effect

In this article we assume a transparent medium. Because of $\chi''_{ij} = 0$ the susceptibility tensor is Hermitian. The same holds true for the (relative) dielectric permittivity $\epsilon_{ij} = \delta_{ij} + \chi_{ij}$, and also for the inverse tensor $(\epsilon^{-1})_{ij}$ which is often used in theoretical optics.

Let us write a Taylor expansion of ϵ^{-1} with respect to quasi-static fields:

$$(\epsilon^{-1})_{ij}(\omega; \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{B}}) = (\epsilon^{-1})^{(0,0)}_{ij}(\omega) \tag{4.339}$$

$$+ (\epsilon^{-1})^{(1,0)}_{ijk}(\omega)\mathcal{E}_k \tag{4.340}$$

$$+ (\epsilon^{-1})^{(0,1)}_{ijk}(\omega)\mathcal{B}_k + \cdots . \tag{4.341}$$

The first term on the right hand side is Hermitian and symmetric, hence real symmetric. We have discussed it in the article on *Crystal Optics*.

The second term describes the action of a quasi-static electric field in linear approximation, if crystal symmetry permits it. The corresponding effects go with the name of Pockels. It is the subject of this article. Following tradition, we denote $(\epsilon^{-1})^{(1,0)}_{ijk}$ by r_{ijk}.

The third term describes the Faraday effect which we discuss in another article.

If crystal symmetry does not allow tensors of rank three with appropriate properties, higher terms must be taken into account, like the Kerr effect, which is bi-linear in the quasi-static electric field.

4.18.3 Crystal Symmetry 3m

If the crystal has an inversion center, such that $\boldsymbol{x} \to -\boldsymbol{x}$ is a symmetry operation, there can be no proper tensor of rank three. The Pockels effect shows up only for non centro-symmetric crystals, such as lithium niobate.

The crystallographic point group of LiNbO_3 is 3m. There is a threefold symmetry axis and a mirror plane. The point group contains the identity

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.342}$$

the reflexion

$$\Pi = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.343}$$

Table 4.3 Multiplication table of the 3m symmetry group made up of the mirror transformation Π and a rotation R by 120° and products thereof

	I	Π	R	R^{-1}	ΠR	$R\Pi$
I	I	Π	R	R^{-1}	ΠR	$R\Pi$
Π	Π	I	ΠR	$R\Pi$	R	R^{-1}
R	R	$R\Pi$	R^{-1}	I	Π	ΠR
R^{-1}	R^{-1}	ΠR	I	R	$R\Pi$	Π
ΠR	ΠR	R^{-1}	$R\Pi$	Π	I	R
$R\Pi$	$R\Pi$	R	Π	ΠR	R^{-1}	I

the rotation

$$R = \begin{pmatrix} -\sqrt{3/4} & \sqrt{3/4} & 0 \\ -\sqrt{3/4} & -\sqrt{1/4} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{4.344}$$

and all of their products. The group 3m is made up of $\{I, \Pi, R, R^{-1}, \Pi R, R\Pi\}$. Table 4.3 describes its structure. You find the product $A \cdot B$ at row A and column B.

We will now construct the most general tensor $r_{ijk} = r_{jik}$ which is compatible with the 3m symmetry group.

4.18.4 Symmetry Compatible Tensors

Let us denote by $\hat{\boldsymbol{c}}$ the unit vector of the three-fold rotation symmetry. This is the z axis of the Cartesian coordinate system. The x, y axes are represented by unit vectors $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$, respectively. Apart from $\hat{\boldsymbol{u}} = \hat{\boldsymbol{x}}$ we define two more unit vectors, namely

$$\hat{\boldsymbol{v}} = -\sqrt{\frac{1}{4}}\hat{\boldsymbol{x}} + \sqrt{\frac{3}{4}}\hat{\boldsymbol{y}} \text{ and } \hat{\boldsymbol{w}} = -\sqrt{\frac{1}{4}}\hat{\boldsymbol{x}} - \sqrt{\frac{3}{4}}\hat{\boldsymbol{y}}. \tag{4.345}$$

Since $\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{v}} = \hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{w}} = \hat{\boldsymbol{w}} \cdot \hat{\boldsymbol{u}} = 1/2$, the angle between them is 120°. Note that $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, $\hat{\boldsymbol{u}}$, $\hat{\boldsymbol{v}}$ and $\hat{\boldsymbol{w}}$ are orthogonal to $\hat{\boldsymbol{c}} = \hat{\boldsymbol{z}}$.

$$\hat{\boldsymbol{x}} \to -\hat{\boldsymbol{x}} \tag{4.346}$$

and a cyclic permutation

$$\hat{\boldsymbol{u}} \to \hat{\boldsymbol{v}} \to \hat{\boldsymbol{w}} \to \hat{\boldsymbol{u}} \tag{4.347}$$

are symmetries. See Fig. 4.15 for a sketch.

We can construct four tensors of rank three which respect 3m symmetry and are symmetric in the first two indexes.

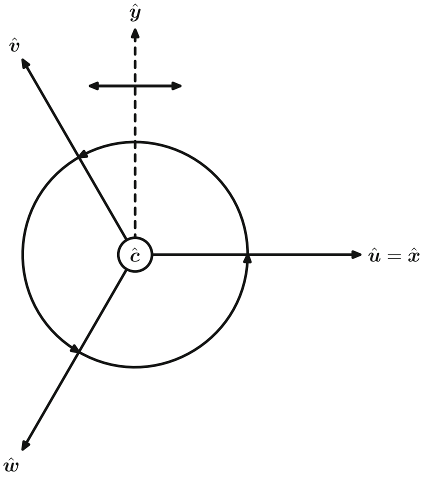

Fig. 4.15 The plane orthogonal to the $\hat{z} = \hat{\boldsymbol{c}}$ axis. $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ as well as $\hat{\boldsymbol{u}}$, $\hat{\boldsymbol{v}}$, $\hat{\boldsymbol{w}}$ are unit vectors. Mirroring with respect to the $\hat{\boldsymbol{y}}, \hat{\boldsymbol{c}}$ plane (or $\hat{\boldsymbol{x}} \to -\hat{\boldsymbol{x}}$) as well as $\hat{\boldsymbol{u}} \to \hat{\boldsymbol{v}} \to \hat{\boldsymbol{w}} \to \hat{\boldsymbol{u}}$ are symmetry operations. These transformations define the 3m space point group

- $\hat{\boldsymbol{c}} \otimes \hat{\boldsymbol{c}} \otimes \hat{\boldsymbol{c}}$ is obviously symmetric in the first pair of indices and respects 3m-symmetry. We obtain

$$D^{(1)}_{ijk} = \hat{c}_i \hat{c}_j \hat{c}_k. \tag{4.348}$$

- $\hat{\boldsymbol{u}} \otimes \hat{\boldsymbol{u}} \otimes \hat{\boldsymbol{c}} + \cdots$ can be simplified because $\hat{\boldsymbol{u}} \otimes \hat{\boldsymbol{u}} + \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}} + \hat{\boldsymbol{w}} \otimes \hat{\boldsymbol{w}}$ is proportional to $\hat{\boldsymbol{x}} \otimes \hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} \otimes \hat{\boldsymbol{y}}$. In components:

$$\hat{u}_i \hat{u}_j + \hat{v}_i \hat{v}_j + \hat{w}_i \hat{w}_j \propto \hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j. \tag{4.349}$$

Our second symmetry complying tensor therefore is

$$D^{(2)}_{ijk} = (\hat{x}_i \hat{x}_j + \hat{y}_i \hat{y}_j) \hat{c}_k. \tag{4.350}$$

- $(\hat{\boldsymbol{u}} \otimes \hat{\boldsymbol{c}} + \hat{\boldsymbol{c}} \otimes \hat{\boldsymbol{u}}) \otimes \hat{\boldsymbol{u}} + \cdots$ can again by simplified by Eq. (4.349). We arrive at

$$D^{(3)}_{ijk} = (\hat{x}_i \hat{c}_j + \hat{c}_i \hat{x}_j) x_k + (\hat{y}_i \hat{c}_j + \hat{c}_i \hat{y}_j) y_k. \tag{4.351}$$

- $\hat{\boldsymbol{u}} \otimes \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{w}}$ is *not* allowed because the expression changes sign upon $\hat{\boldsymbol{x}} \to -\hat{\boldsymbol{x}}$. However, if we replace $\hat{\boldsymbol{u}}$ by $\hat{\boldsymbol{u}}' = \hat{\boldsymbol{c}} \times \hat{\boldsymbol{u}}$ and likewise for $\hat{\boldsymbol{v}}$ and $\hat{\boldsymbol{w}}$, then $\hat{\boldsymbol{u}}' \otimes \hat{\boldsymbol{v}}' \otimes \hat{\boldsymbol{w}}'$ does not acquire this minus sign. Hence we should try the expression

$$(\hat{\boldsymbol{u}}' \otimes \hat{\boldsymbol{v}}' + \hat{\boldsymbol{v}}' \otimes \hat{\boldsymbol{u}}') \otimes \hat{\boldsymbol{w}} + \text{cyclic permutations.} \tag{4.352}$$

This *ansatz* is symmetric in the first index pair and obeys 3m symmetry. It is proportional to $(\hat{\boldsymbol{x}} \otimes \hat{\boldsymbol{y}} + \hat{\boldsymbol{y}} \otimes \hat{\boldsymbol{x}}) \otimes \hat{\boldsymbol{x}} + (\hat{\boldsymbol{x}} \otimes \hat{\boldsymbol{x}} - \hat{\boldsymbol{y}} \otimes \hat{\boldsymbol{y}}) \otimes \hat{\boldsymbol{y}}$. The fourth (and last) symmetry complying tensor is

$$D^{(4)}_{ijk} = (\hat{y}_i \hat{y}_j - \hat{x}_i \hat{x}_j) \hat{y}_k - (\hat{x}_i \hat{y}_j + \hat{y}_i \hat{x}_j) \hat{x}_k. \tag{4.353}$$

Table 4.4 Pockels coefficients for lithium niobate in pmV^{-1}. The first column shows the constants of Eq. (4.354), the second in standard notation. The tensor entries in the third column are equal to r_a. The fourth and fifth column are measured values at constant stress and constant strain, respectively, for light of a helium-neon laser

r_a	Also	r_{ijk}	Free	Clamped
r_1	r_{33}	r_{333}	30.9	30.8
r_2	r_{13}	$r_{113} = r_{223}$	9.6	8.6
r_3	r_{51}	$r_{131} = r_{311} = r_{232} = r_{322}$	32.6	28.0
r_4	r_{22}	$r_{222} = -r_{121} = -r_{211} = -r_{112}$	6.8	3.4

The symmetry in the first pair of indexes as well as the mirror symmetry are obvious; the symmetry with respect to 120° rotations is guaranteed by adding cyclic permutations.

The tensor of Pockels coefficients can be written as

$$r_{ijk}(\omega) = \sum_{a=1}^{4} r_a(\omega) D^{(a)}_{ijk}. \tag{4.354}$$

Table 4.4 lists the non-vanishing tensor elements. The last two columns are values for lithium niobate, for constant stress (free) or constant strain (clamped). The former refer to slowly varying external fields $\mathcal{E}$ when stress can follow strain. The clamped values are applicable if $\mathcal{E} = \mathcal{E}(f)$ changes so rapidly with frequency f that there is no time for achieving elastic equilibrium. The listed values from [5] are for He-Ne laser light, $\lambda = 632.8\,\text{nm}$.

4.18.5 Digression on Orders of Magnitude

The Pockels coefficients are some 10 pmV^{-1}. Are such values arbitrary, GOD given? No, as we will argue in this digression on atomic units. After all, solid state physics is based on quantum theory. In particular, a solid is idealized as an ensemble of nuclei and their electrons. It is a good approximation to idealize the solid as a lattice of fixed ions and a cloud of shared electrons which interact via Coulomb forces. The following constants of nature (or conventions on the system of units) enter the game. There is e, the charge of the proton and, with a negative sign, of the electron. Ordinary matter cannot be understood without the laws of quantum mechanics, hence $\hbar$ shows up. The mass m of electrons will be found and the factor $4\pi\epsilon_0$ which appears in the Coulomb force law. Atomic units are combinations[42] $e, m, \hbar$ and $4\pi\epsilon_0$ for given physical quantities, such as time, length, voltage, electric field strength and so on. The atomic unit of electric field strength is

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[42] products of powers of

$$\mathcal{E}^{\star} = \frac{m^2 e^5}{(4\pi\epsilon_0)^3 \hbar^4} = 0.514 \times 10^{12}\ \mathrm{Vm}^{-1}. \tag{4.355}$$

Measured in atomic units, $r_{333}\,\mathcal{E}^{\star} \approx 16$ (free) is reasonably large. Lithium niobate is rather resilient to quasi-static external fields. See the article on *Natural Units* where we discuss more examples.

4.18.6 How Light Propagation is Affected

Let us first apply an electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}\hat{\boldsymbol{c}}$ along the optical axis. According to Table 4.4 we find

$$\epsilon^{-1} = \begin{pmatrix} \frac{1}{n_\mathrm{o}^2} + r_{13}\,\mathcal{E} & 0 & 0 \\ 0 & \frac{1}{n_\mathrm{o}^2} + r_{13}\,\mathcal{E} & 0 \\ 0 & 0 & \frac{1}{n_\mathrm{e}^2} + r_{33}\,\mathcal{E} \end{pmatrix}. \tag{4.356}$$

Here, $n_\mathrm{o} = 2.286$ is the refractive index of the ordinary and $n_\mathrm{e} = 2.200$ of the extraordinary beam.[43] See the article on *Crystal Optics*. Since the electric field strength is always very small as compared with the atomic unit thereof, we may write

$$n_\mathrm{o}(\mathcal{E}) = n_\mathrm{o} - \frac{1}{2} n_\mathrm{o}^3\, r_{13}\,\mathcal{E} \text{ and } n_\mathrm{e}(\mathcal{E}) = n_\mathrm{e} - \frac{1}{2} n_\mathrm{e}^3\, r_{33}\,\mathcal{E}. \tag{4.357}$$

Ordinary or extraordinary beams remain ordinary or extraordinary. However, their propagation constants now depend linearly on the external electric field strength. When propagating a distance ℓ, there is a phase shift of $\phi = -n^3 r \mathcal{E}\ell/2$ which may be employed for modulating or switching light or for measuring phase shifts, such as in fiber gyros.

We now discuss an electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}\hat{\boldsymbol{x}}$ in x direction, perpendicular to the optical axis. The inverse dielectric permittivity is

$$\epsilon^{-1} = \begin{pmatrix} \frac{1}{n_\mathrm{o}^2} & -r_{22}\,\mathcal{E} & r_{51}\,\mathcal{E} \\ -r_{22}\,\mathcal{E} & \frac{1}{n_\mathrm{o}^2} & 0 \\ r_{51}\,\mathcal{E} & 0 & \frac{1}{n_\mathrm{e}^2} \end{pmatrix}. \tag{4.358}$$

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[43] For He-Ne laser light, from [5].

Likewise, if the electric field is $\boldsymbol{\mathcal{E}} = \mathcal{E}\hat{\boldsymbol{y}}$, one obtains

$$\epsilon^{-1} = \begin{pmatrix} \frac{1}{n_{\mathrm{o}}^2} - r_{22}\,\mathcal{E} & 0 & 0 \\ 0 & \frac{1}{n_{\mathrm{o}}^2} + r_{22}\,\mathcal{E} & r_{51}\,\mathcal{E} \\ 0 & r_{51}\,\mathcal{E} & \frac{1}{n_{\mathrm{e}}^2} \end{pmatrix}. \tag{4.359}$$

The situation is rather complicated, and we shall not discuss it further.

To summarize: If the external electric field is parallel to the optical axis of a lithium niobate crystal, it remains optically uniaxial. Its ordinary and extraordinary indexes of refraction change linearly with the applied field strength. If the external electric field is perpendicular to the optical axis, the medium becomes optically biaxial.

4.18.7 Kerr Effect

By the so-called totalitarian principle[44] of physics, crystals which lack an inversion center always show the Pockels effect. However, if there is an inversion center, the quasi-static external electric field $\boldsymbol{\mathcal{E}}$ will modify the susceptibility only in second order. This so called Kerr effect is quite normal, it does not require a special crystal symmetry. In fact, it shows up even for optically isotropic media, such as liquids or cubic crystals. Traditionally, the Kerr constant R is defined as

$$(\epsilon^{-1})^{(2,0)}_{ijkl} = R\delta_{ik}\delta_{jl} \tag{4.360}$$

in the notation of Eq. (4.339), or by

$$(\epsilon^{-1})_{ij} = \frac{1}{n^2}\delta_{ij} + R\mathcal{E}_i\mathcal{E}_j. \tag{4.361}$$

A contribution proportional to $\delta_{ij}\delta_{kl}$ would simply modify the refractive index n by a tiny amount, an effect which is difficult to detect.

Assume the electric field pointing in 3-direction, $\mathcal{E}_1 = \mathcal{E}_2 = 0$ and $\mathcal{E}_3 = \mathcal{E}$. The dielectric permittivity tensor will be

$$\epsilon = \begin{pmatrix} n_{\mathrm{o}}^2 & 0 & 0 \\ 0 & n_{\mathrm{o}}^2 & 0 \\ 0 & 0 & n_{\mathrm{e}}^2 \end{pmatrix}, \tag{4.362}$$

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[44] *Everything not forbidden is compulsory.*

with the ordinary index of refraction $n_\mathrm{o} = n$ and an extraordinary refractive index

$$n_\mathrm{e} = n - \frac{1}{2} n^3 R \mathcal{E}^2. \tag{4.363}$$

The material becomes birefringent, the optical axis being the direction of the quasi-static external electric field $\boldsymbol{\mathcal{E}}$. The birefringence $n_\mathrm{o} - n_\mathrm{e}$ grows quadratically with the field strength.

In a liquid, the quasi-static electric field partially orders molecules with a dipole moment, thereby making it optically uniaxial. The effect is particularly large for nitrobenzene,[45] namely $R = 1.50 \times 10^{-18}\,\mathrm{m^2\,V^{-2}}$. If an electric field of $10\,\mathrm{kV\,cm^{-1}}$ is applied, the birefringence is $\Delta n = 2.8 \times 10^{-6}$. The phase shift between the ordinary and the extraordinary beam will be $\pi/2$ if they propagate a distance of 5.7 cm.

In a Kerr cell, the linearly polarized light beam propagates along the x axis. When entering the cell, its electric field shall be $\boldsymbol{E} \propto (0, 1, 1)$, a superposition of an ordinary and an extraordinary beam. Have a look at Fig. 4.5. Both propagate with slightly different propagation constants, and after a certain length the field will be $\boldsymbol{E} \propto (0, 1, -1)$. When leaving the Kerr cell, the polarization vector has changed from $+45°$ to $-45°$. Suitably arranged polarizers will make sure that light passes the Kerr cell. If, however, the electric field is switched off, the beam may not pass the arrangement of a Kerr cell and the polarizers before and after it. The Kerr effect allows to switch a light beam by a voltage. Since this is a book on materials, not on devices, we cannot pursue this thread any further.

4.19 Reactions and Diffusion

Diffusion of one kind of particles in a gas, a liquid, or a solid is a simple problem. We have discussed it already in our article on *Brownian Motion*. Moreover, the diffusion equation for one species of particles is formally similar to the heat equation. After all, heat conduction is nothing else but phonon diffusion. Things become really interesting if two or more species of particles diffuse which locally undergo chemical reactions. Although the diffusion equations are linear in the concentrations of the involved particles, their interactions are described by non-linear relations between them. Thus, the combination of localized chemical reactions and diffusion leads to non-linear systems of partial differential equations, the solutions of which show remarkable features, for instance spontaneous pattern formation. This article is intended to be an introduction into an entirely new world of phenomena.

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[45] Kaye and Laby [5], for He-Ne laser light.

4.19.1 Gray-Scott Model

Among hundreds of possible examples we concentrate on the Gray-Scott [1] model because it is simple and yet full of surprising details. There are two species of particles, U and V. U serves as a substrate. In an auto-catalytic reaction it is transformed into V by U+2V → 3V. New U particles enter the reaction region by passing through a membrane, and V particles pass outside through the same membrane.

Denote by $u = u(x, y)$ and $v = v(x, y)$ the concentration of U and V particles, respectively. The production rate per unit volume of U particles is

$$\pi^{\mathrm{u}} = -Ruv^2 + F(\bar{u} - u). \tag{4.364}$$

The first term on the right hand side takes the mass action law into account. One U and two V must come into close contact to allow for a chemical reaction. The rate therefore is proportional to the first power of u and the second power of v. Any such reaction removes a U particle, therefore the minus sign. R is a positive constant. The second term formulates that the inflow of U particles is proportional to the difference between the constant concentration $\bar{u}$ outside and the concentration u inside the reactor. F is a positive constant.

For the volumetric production rate of V particles we write

$$\pi^{\mathrm{v}} = +Ruv^2 - (F + K)v. \tag{4.365}$$

Any reaction U+2V → 3V adds one V particle, therefore the $+Ruv^2$ contribution. V particles passing out of the reactor are removed, that is, $\bar{v} = 0$ outside. The outflow of V particles therefore is proportional to v, the proportionality constant $F + K$ may differ from F for the inflow of U particles.

The Gray-Scott model combines this local reaction mechanism with diffusion, which is described by

$$\partial_t u = D_{\mathrm{U}} \Delta u + \pi^{\mathrm{u}} \text{ and } \partial_t v = D_{\mathrm{V}} \Delta v + \pi^{\mathrm{v}}. \tag{4.366}$$

$\Delta = \partial_x \partial_x + \partial_y \partial_y$ is the Laplacian in two dimensions. D_{U} and D_{V} are the diffusion constants for U and V particles, respectively. Although Eq. (4.366) with Eqs. (4.364) and (4.365) appear to be simple, these equations describe a huge manifold of solutions which critically depend on the model parameters.

4.19.2 Similarity Considerations

Let us introduce a typical time t_* and a typical length ℓ_*. We introduce a dimensionless time by $t = t_* \hat{t}$, dimensionless coordinates by $x = \ell_* \hat{x}$ and $y = \ell_* \hat{y}$. The concentration of U particles can be written as $u(t, x, y) = \bar{u}\, \hat{u}(\hat{t}, \hat{x}, \hat{y})$

while the distribution of V particles is described by $v(t,x,y) = \bar{u}\,\hat{v}(\hat{t},\hat{x},\hat{y})$. All headed symbols are dimension-less. Differentiation with respect to time becomes $\partial_t = \hat{\partial}_t / t_*$, and the Laplacian is $\Delta = \hat{\Delta}/\ell_*^2$.

Let us rewrite Eq. (4.366):

$$\hat{\partial}_t \hat{u} = \frac{t_* D_{\mathrm{U}}}{\ell_*^2} \hat{\Delta}\hat{u} - t_* \bar{u}^2 \hat{u}\hat{v}^2 + t_* F(1-\hat{u}) \tag{4.367}$$

and

$$\hat{\partial}_t \hat{v} = \frac{t_* D_{\mathrm{V}}}{\ell_*^2} \hat{\Delta}\hat{v} + t_* \bar{u}^2 \hat{u}\hat{v}^2 - t_*(F+K)\hat{v}. \tag{4.368}$$

We choose t_* and ℓ_* such that

$$\frac{t_* D_{\mathrm{U}}}{\ell_*^2} = 1 \text{ and } t_* R\bar{u}^2 = 1, \tag{4.369}$$

and we denote $D_{\mathrm{U}}/D_{\mathrm{V}}$ by σ, $t_* F$ by f, and $t_* K$ by k. Dropping the heads over symbols we arrive at

$$\partial_t u = \Delta u - uv^2 + f(1-u) \tag{4.370}$$

and

$$\partial_t v = \frac{1}{\sigma}\Delta v + uv^2 - (f+k)v. \tag{4.371}$$

All quantities in Eqs. (4.370) and (4.371) are now dimension-less. The Gray-Scott model contains three parameters, the ratio σ of diffusion constant, the inflow factor f of U particles and the outflow factor $f+k$ for V particles.[46]

4.19.3 Homogeneous Solutions

Physical intuition says that any solution of Eqs. (4.370) and (4.371) will converge, with $t \to \infty$, towards a stationary and homogeneous particle distribution. After all, diffusion tends to smooth spatial inhomogeneities. So we look for solutions $u(t,x,y) = u$ and $v(t,x,y) = v$, for particle concentrations, which neither depend on time t nor on location (x,y). The Gray-Scott model (4.370), Eq. (4.371) reduces to

$$uv^2 = f(1-u) \text{ and } uv^2 = (f+k)v. \tag{4.372}$$

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[46] See Pearson [9].

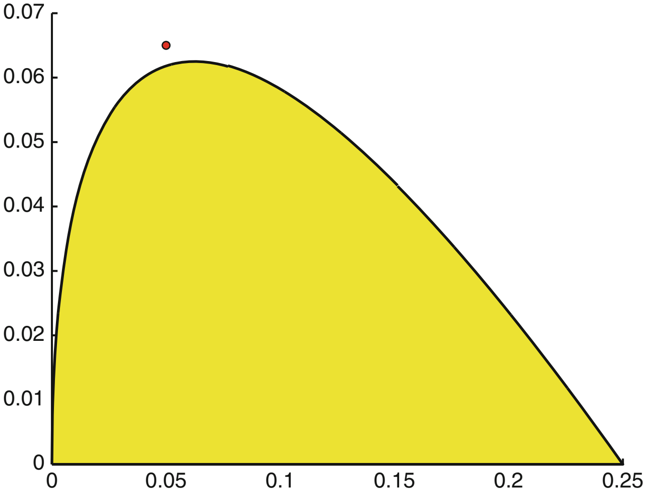

Fig. 4.16 Parameters of the Gray-Scott model. f from *left* to *right*, k from *bottom* to *top*. Parameters in the marked region allow for two stationary homogeneous solutions $(u_\pm, v_\pm)$ besides $(1, 0)$. The *dot* marks a parameter set for which we later will show a solution

One solution is evident, namely $u = 1$ and $v = 0$. The concentration of U and V particles outside and inside the reaction region are the same. There are, however, another two solutions, namely

$$u_\pm = \frac{1}{2} \pm \sqrt{\frac{1}{4} - \frac{(f+k)^2}{f}} \text{ with } v_\pm = \frac{f}{f+k}(1 - u_\pm). \tag{4.373}$$

These additional stationary homogeneous solutions do not exist for all parameter sets f and k, but only if

$$f \geq 0\,,\ (f+k) \geq 0 \text{ and } f \geq 4(f+k)^2 \tag{4.374}$$

hold true. This delimits the parameter space to

$$f \geq 0 \text{ and } -f \leq k \leq \frac{\sqrt{f}}{2} - f. \tag{4.375}$$

It is usually assumed that U particles pass the membrane more easily than V particles. This is expressed by $k \geq 0$. Then the parameter space is further restricted to

$$f \geq 0 \text{ and } 0 \leq k \leq \frac{\sqrt{f}}{2} - f. \tag{4.376}$$

We have plotted this region in Fig. 4.16.

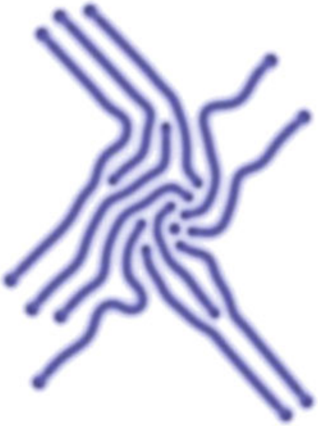

Fig. 4.17 The Gray-Scott model has been solved with $\sigma = 2$, $f = 0.050$ and $k = 0.065$. These parameters correspond to the mark in Fig. 4.16. The partial differential equation has been equipped with arbitrary initial conditions. This is an early development stage. Worm-like regions expand, but avoid each other. They have not yet met the boundary. White corresponds to low V, but high U concentration

4.19.4 Pattern Formation

The diffusion equations (4.370) and (4.371) for $u = u(t,x)$ and $v = v(t,x)$ must be supplemented by an initial and by boundary conditions. The reaction region is described by the square $0 \le x \le 1$ and $0 \le y \le 1$. In order to simulate translational invariance, periodic boundary conditions are usually imposed:

$$u(t,0,y) = u(t,1,y) \text{ as well as } u(t,x,0) = u(t,x,1), \tag{4.377}$$

and the same for $v(t,x,y)$. The initial fields $u_0(x,y) = u(0,x,y)$ and $v_0(x,y) = v(0,x,y)$ should respect Eq. (4.377).

We refrain from describing a problem solver. There are many to be found in the Internet. With one of them, a Java applet, we have produced the following pictures.[47] You may specify the parameters f and k, and the program shows a sequence of u-fields as they develop with time. Initial conditions are either random or standard. Figure 4.17 is an example.

The next picture Fig. 4.18 shows the solution at an intermediate state of evolution. Some worms have met the boundary and thus reappear on the opposite side. This is a consequence of imposing unphysical periodic boundary conditions which, however, warrant translation symmetry. You cannot mimic the infinite $x - y$ plane by a necessarily finite mesh on a computer.

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[47] http://www.aliensaint.com/uo/java/rd/ by Jonathan Lidbeck while he was with the University of Oregon.

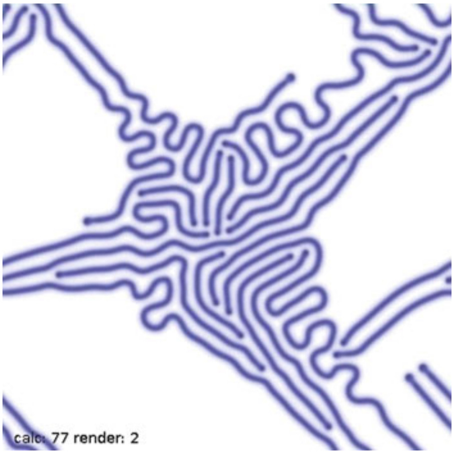

Fig. 4.18 See the caption of Fig. 4.17. The concentration of U particles is shown at an intermediate state of pattern development

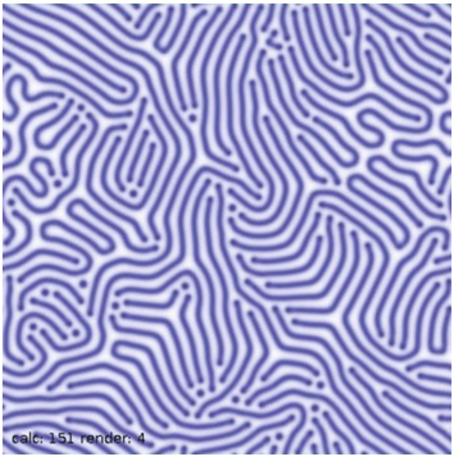

Fig. 4.19 See the caption of Fig. 4.17. This picture displays $u(t, x, y)$ for $t \to \infty$. In the vicinity of parameters $\sigma = 2$, $f = 0.050$ and $k = 0.065$ there are non-trivial stationary patterns of which this is an example

The parameter set $\sigma = 2$, $f = 0.050$ and $k = 0.065$ leads to a stationary pattern which we show in Fig. 4.19.

For other parameters one will encounter completely different solutions. Some never converge with time. In other occasions, there is a definite pattern which however oscillates or moves. There are parameter sets for which dots grow into small worms which soon split into two other dots resembling bacteria colonies.

4.19.5 Further Remarks

Models like that of Gray and Scott play an important role in theoretical biology. It was Alan Turing's seminal paper on *The Chemical Basis of Morphogenesis* [13] where local non-linear reactions and diffusion were combined for the first time in order to explain forms and patterns. There are stable or quasi-stable states far away from thermodynamic equilibrium. In this article we cannot go beyond striving the vast and growing field of research on non-linear phenomena. Simple and plain equations, such as for diffusion with local non-linear reactions or the Navier-Stokes equation promise surprises for years to come.

4.20 Reynold's Number

Fluids, that is liquids or gases, are characterized by the absence of elastic shear stress. A rather large class of fluids are well described by the non-linear Navier-Stokes equations for a Newtonian fluid or a variation thereof. Water and air are among them. Stationary solutions of the Navier-Stokes equation may be scaled provided the dimension-less Reynold number `Re` remains unchanged.

4.20.1 Navier-Stokes Equation

The famous Navier-Stokes equation is nothing else but the momentum balance equation for fluid media with Newton's friction law. We will further specialize to an incompressible fluid, such as water.

The momentum balance equation is

$$\partial_t \varrho v_i + \partial_j \{ \varrho v_i v_j - T_{ij} \} = f_i . \tag{4.378}$$

Here ϱ is the mass density, v_i denotes the center-of-mass flow velocity, T_{ij} the stress tensor and f_i is the external force per unit volume. The flow of momentum P_i in direction j has been split into the convection term $\varrho v_i v_j$ and the conduction contribution $-T_{ij}$. f_i is the production rate of momentum P_i per unit volume.

The stress tensor must be split into an elastic and an inelastic contribution, $T_{ij} = T'_{ij} + T''_{ij}$, respectively. The elastic, or reversible part is

$$T'_{ij} = -p\,\delta_{ij} \tag{4.379}$$

for a fluid medium. There are no off-diagonal elements, or shear forces. p is the pressure. The inelastic, or irreversible part of the stress tensor, for a Newtonian fluid, is

$$T''_{ij} = \eta\,\{\partial_i v_j + \partial_j v_i\}. \tag{4.380}$$

This expression guaranties that the stress tensor be symmetric upon exchange of indexes. It formulates the idea that friction is proportional to velocity differences of neighboring material points. $\eta = \eta^{\mathrm{s}}$ is the shear viscosity of the fluid.

Let us further specialize to incompressible fluids, such as water. They are characterized by a constant mass density which, because of $\partial_t \varrho + \partial_i \varrho v_i = 0$ (conservation of mass) implies

$$\partial_i v_i = 0. \tag{4.381}$$

Baking all this together gives

$$\varrho(\partial_t v_k + v_i \partial_i v_k) = \varrho\,\mathrm{D}_t\, v_k = -\partial_k p + \eta \Delta v_k + f_k, \tag{4.382}$$

the Navier-Stokes equation. D_t denotes the substantial time derivative as felt by a co-moving observer. The reason for the acceleration of a material point is a negative pressure gradient, friction, and an external force such as gravitation or a Coriolis force.

4.20.2 Similarity Considerations

External forces are usually not important in hydrodynamic problems, so we drop the last term in Eq. (4.382). We choose a typical length ℓ_* and a typical velocity v_*. True lengths are written as $\ell = \hat{\ell}\ell_*$, true velocities as $v = \hat{v}v_*$. Likewise, we measure time in units of $t_* = \ell_*/v_*$ and pressure in units of $p_* = \varrho v_*^2$. With these conventions, the Navier-Stokes equation (4.382) formally simplifies to

$$\hat{\partial}_t \hat{v}_k + \mathtt{Re}\, \hat{v}_i \hat{\partial}_i \hat{v}_k = -\hat{\partial}_k \hat{p} + \hat{\Delta} \hat{v}_k. \tag{4.383}$$

$\mathtt{Re}$ stands for Reynold's number

$$\mathtt{Re} = \frac{\varrho v_* \ell_*}{\eta}. \tag{4.384}$$

You should check the physical dimensions to convince yourself that $\mathtt{Re}$ is indeed a dimension-less number. The Navier-Stokes equation (4.383) is entirely dimensionless, hence ready for numerical studies. Problems with differing ℓ_* and v_* but the same Reynold number are described by one and the same equation. This allows for simulating real-world problems on small scales. If a ship is modeled ten to one and the velocity is increased by a factor of ten, the same dimension-less solution describes both situations.

4.20.3 Laminar Flow and Turbulence

Physicists like linear problems because they are easy to solve. On the other hand, non-linearities produce interesting and surprising effects. The Navier-Stokes equation contains `Re` as a parameter which continuously changes the equation's behavior: from linear to slightly non-linear to highly non-linear, from creeping to laminar to turbulent.

It is the second term in Eq. (4.383) which is problematic. It may vanish because Reynold's number is very small such that $\mathtt{Re}\,\hat{v}_i\,\hat{\partial}_i\,\hat{v}_k$ may safely be neglected. We then speak of a laminar flow because layers[48] glide one upon the other with slightly different velocities. Our article on *Stoke's Law* explicitly relies on $\mathtt{Re} \ll 1$.

However, the term $\mathtt{Re}\,\hat{v}_i\,\hat{\partial}_i\,\hat{v}_k$ may also vanish because of symmetry reasons. See the article on the *Hagen-Poiseuille Law*. Although there is a plausible solution, it may be unstable if Reynold's number is large enough. How large `Re` must be in order to cause turbulence depends very much on details. The transition from laminar to turbulent flow may be triggered by small obstacles or any kind of surface roughness. Although much has been said about turbulence, the phenomenon is still more or less mysterious. This is so because the velocity field depends critically on initial and boundary conditions such that an impression of randomness springs to mind. The larger Reynold's number, the more so.

Horace Lamb, a renowned researcher in hydrodynamics, reportedly [7] said in an address to the British Association for the Advancement of Science: "I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic". Also Richard Feynman called turbulence "the most important unsolved problem of classical physics" [7].

4.21 Sound in Air

Think about a small region with mass M within a gas in equilibrium. If this region is compressed, there will be a counter force, or pressure, to re-establish equilibrium. Since the region has mass, the volume then, because of inertia, becomes too large, and a compressing counter pressure tries to bring it back to equilibrium. For small deviations from equilibrium, the pressure will be proportional to the volume deviation from its equilibrium value. These are the ingredients of a harmonic oscillation. Since the pressure gradients drives a flow of momentum, the oscillation will propagate from site to site, and we expect pressure deviations to be governed by a wave equation. In the following we derive the sound wave equation, describe a

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[48] Latin *lamina*, layer.

very simple sound source, discuss acoustic energy and present the classical formula for sound attenuation.

4.21.1 Wave Equation

Let us denote by $\bar{p}$, $\bar{\varrho}$ and $\bar{v}_i = 0$ the equilibrium values of pressure, mass density and center of mass velocity. We write $p = \bar{p} + \tilde{p}$, $\varrho = \bar{\varrho} + \tilde{\varrho}$ and $v_i = \tilde{v}_i$ for the actual pressure, mass density and velocity of material points. In this article we shall study small deviations[49] from equilibrium only. All equations will be linear in deviations $\tilde{x}$.

The mass balance equation now reads

$$\partial_t \tilde{\varrho} + \bar{\varrho} \partial_i \tilde{v}_i = 0. \tag{4.385}$$

The momentum balance equation with $T_{ij} = -\delta_{ij} p$ becomes

$$\bar{\varrho} \partial_t \tilde{v}_i + \partial_i \tilde{p} = 0. \tag{4.386}$$

External forces, such as gravitation, play no role here. The term $\partial_j \varrho v_i v_j$ is of second and higher order and has been dropped. The divergence of Eq. (4.386) is

$$\bar{\varrho} \partial_t \partial_i \tilde{v}_i + \Delta \tilde{p} = 0. \tag{4.387}$$

We insert Eq. (4.385) and arrive at

$$-\partial_t^2 \tilde{\varrho} + \Delta \tilde{p} = 0. \tag{4.388}$$

This equation applies to all weekly perturbed fluid media. To proceed, we need a relation between the deviations $\tilde{p}$ of pressure and $\tilde{\varrho}$ of mass density.

Unfortunately, the ideal gas law[50]

$$p = \frac{\varrho}{M} R T \tag{4.389}$$

does not help. For deviations it reads

$$\tilde{p} = \frac{\tilde{\varrho}}{M} R T + \frac{\varrho}{M} R \tilde{T}, \tag{4.390}$$

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[49] In this article the tilde does not denote the Fourier transform, but a small deviation from the equilibrium value.

[50] M is the molar mass of air and R denotes the universal gas constant.

it just would introduce another field, namely the temperature deviation $\tilde{T}$ from the equilibrium value.

In our article on a *Model Atmosphere* we have studied the free energy of a diatomic ideal gas which describes air very well. We could show that two states—labeled by 1 and 2—have the same entropy if

$$\frac{T_1}{T_2} = \left\{\frac{V_1}{V_2}\right\}^{-2/5} = \left\{\frac{\varrho_1}{\varrho_2}\right\}^{2/5} = \left\{\frac{p_1}{p_2}\right\}^{2/7} \tag{4.391}$$

holds true. With $\varrho_1 = \bar{\varrho} + \tilde{\varrho}$, $\varrho_2 = \bar{\varrho}$ and the same for pressure we find

$$\tilde{\varrho} = \frac{5}{7}\frac{\bar{\varrho}}{\bar{p}}\,\tilde{p} = \frac{1}{c^2}\,\tilde{p}, \tag{4.392}$$

where c^2 is an abbreviation for

$$c^2 = \frac{7}{5}\frac{\bar{p}}{\bar{\varrho}} = \frac{7}{5}\frac{R\bar{T}}{M}. \tag{4.393}$$

We insert this relation into Eq. (4.388) and obtain

$$\left\{\frac{1}{c^2}\partial_t^2 - \Delta\right\}\tilde{p} = 0, \tag{4.394}$$

a wave equation. Bear in mind that Eq. (4.394) is the result of linearizing various balance and material equations. Also note that the mass density fluctuation obeys the same wave equation since $\tilde{\varrho}$ and $\tilde{p}$ are proportional.

The constant c of Eq. (4.393) is obviously the speed of sound in a diatomic ideal gas. For T = 20 °C and with $R = 8.314\ \mathrm{J\,K^{-1}\,mol^{-1}}$ and $M = 0.02897\ \mathrm{kg\,mol^{-1}}$ we calculate $c = 343\,\mathrm{m\,s^{-1}}$ as the speed of sound in dry air. In dry air, because a substantial amount of water vapor is not compatible with the assumption of a gas of diatomic molecules.

The wave equation (4.394) applies to liquids as well. The only difference is that the speed of sound is given by

$$c^2 = \left(\frac{\partial p}{\partial \varrho}\right)_S. \tag{4.395}$$

The dependency of pressure on the mass density at constant entropy cannot be calculated so easily. Kaye and Laby [5] cite $c = 1,522\ \mathrm{m\,s^{-1}}$ for sea water at 20 °C.

4.21.2 Sound Generation

Let us discuss a very simple mechanism for exciting a sound wave. We assume a pulsating sphere of radius $R(t) = R_0 + A\cos\omega t$. The radius oscillates harmonically between $R_0 + A$ and $R_0 - A$. A is the amplitude of radius oscillation, a real number. It is supposed to be small if compared with R_0.

The displacement at the sphere's surface is

$$\tilde{u}_i(t, R_0\boldsymbol{n}) = An_i\,\mathrm{e}^{-\mathrm{i}\omega t}\,, \tag{4.396}$$

the velocity there

$$\tilde{v}_i(t, R_0\boldsymbol{n}) = -\mathrm{i}\omega\,An_i\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{4.397}$$

Here $\boldsymbol{n} = \boldsymbol{x}/R_0$ is the surface normal vector. In these and in the following equations always the real part is understood such that displacement, velocity, mass density and pressure are real. For the mass density oscillation we find, with Eqs. (4.385) and (4.392), the expression

$$\tilde{\varrho}(t, R_0\boldsymbol{n}) = 3\bar{\varrho}\frac{A}{R_0}\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{4.398}$$

Hence the pressure oscillation at the sphere's surface is

$$\tilde{p}(t, R_0\boldsymbol{n}) = 3\bar{\varrho}\frac{A}{R_0}c^2\,\mathrm{e}^{-\mathrm{i}\omega t} = 3\bar{p}\frac{A}{R_0}\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{4.399}$$

We look for a spherically symmetric solution of the wave equation (4.394) which vanishes at infinity. Here it is:

$$\tilde{p}(t, r\boldsymbol{n}) = B\,\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\,\mathrm{e}^{-\mathrm{i}\omega t} \quad \text{with } k = \frac{\omega}{c}. \tag{4.400}$$

The boundary condition (4.399) demands

$$B = 3\bar{p}\,\mathrm{e}^{-\mathrm{i}kR_0}A, \tag{4.401}$$

so that the solution is

$$\tilde{p}(t, r\boldsymbol{n}) = 3\bar{p}\,\frac{A}{r}\,\mathrm{e}^{\mathrm{i}k(r-R_0)}\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{4.402}$$

Recall: the sphere with radius R_0 pulsates with amplitude A and angular frequency $\omega = ck$. $\bar{p}$ denotes the average pressure, $\tilde{p} = \tilde{p}(t, r\boldsymbol{n})$ the deviation from it at time t and distance $r \geq R_0$ from the center of the pulsating sphere. The solution is spherically symmetric because the direction unit vector $\boldsymbol{n}$ does not appear on the right hand side of Eq. (4.400).

Energy

The energy related with sound is neither potential nor internal, but kinetic. Its current density is given by

$$j_i(E^{\mathrm{k}}) = S_i = -v_k T_{ki} = p v_i , \tag{4.403}$$

for a fluid medium. Let us calculate it for the example of a pulsating sphere as discussed above. Then $S_i = \tilde{p}\tilde{v}_i$ in linear approximation (if time averaged).

From Eq. (4.402) we calculate, by Eq. (4.385), the following expression:

$$\tilde{v}_i(t, r\boldsymbol{n}) = \frac{3\bar{p}}{\bar{\varrho}\omega} \left\{ k + \frac{\mathrm{i}}{r} \right\} \frac{A}{r} \, \mathrm{e}^{\mathrm{i}k(r - R_0)} \, \mathrm{e}^{-\mathrm{i}\omega t} \, n_i , \tag{4.404}$$

or

$$\tilde{v}_i(t, r\boldsymbol{n}) = \frac{1}{c\bar{\varrho}} \left\{ 1 - \frac{1}{\mathrm{i}kr} \right\} \tilde{p}(t, r\boldsymbol{n}) \, n_i . \tag{4.405}$$

Now, the factor in front of $\tilde{p}$ is complex. Its real part defines the velocity variation which is in phase with pressure oscillations, the imaginary part describes a 90° phase shift. Therefore, the energy current density is proportional to $1/r^2$,

$$\boldsymbol{S}(t, r\boldsymbol{n}) = \frac{P}{4\pi r^2} \boldsymbol{n}, \tag{4.406}$$

where

$$P = \int_{r=R_0} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{S} \tag{4.407}$$

is the power fed into the acoustic wave by the pulsating sphere.

Equations (4.402) and (4.405) are exact solutions to the linearized balance equations of mass and momentum for a fluid medium without dissipation and heat conduction. Equation (4.405) beautifully shows the distinction between the near field ($1/kr$ cannot be neglected) and the far field ($1/kr \approx 0$).

A pulsating ball is the most simple sound source. Loudspeakers are more refined. Sound may also be generated by vibrating parts of a car's engine or body or by turbulent flow of air, by musical instruments, by the vocal cords, by transducers relying on the piezoelectric effect and so forth.

Attenuation

Equation (4.406) is a typical result: the energy of an outgoing wave, if integrated over a sphere of radius r, does not depend on the distance r from the source.

This finding, namely wave energy conservation, is an idealization. In fact, there is an irreversible transfer from kinetic energy into internal energy. Two mechanisms are responsible for the attenuation of sound waves. They can be traced back to two simplifications we have introduced earlier.

The attenuation of sound waves is *not* due to the linear approximation. Otherwise, weak waves should be damped less than stronger waves, which is not true.

We have derived the wave equation (4.394) with a stress tensor $T_{ij} = -p\delta_{ij}$, where p is the pressure. This, however, is only half the truth. The stress tensor consists of a reversible part—which we have taken into account—and an irreversible contribution which describes internal friction and has been neglected so far. It will be linear in the velocity gradient.

We have also assumed that the compressibility is to be calculated for constant entropy which boils down to neglecting heat conduction. If heat conduction is to be included, the balance equation for entropy comes into the game. The temperature field couples to the pressure field in such a way that sound waves are damped.

Quite formally, the dispersion relation $\omega = \omega(\boldsymbol{k})$ will acquire small imaginary terms such that, for given angular frequency ω, the corresponding wave vector $\boldsymbol{k}$ is no longer real. In fact, its imaginary part produces an $\mathrm{e}^{-\alpha z}$ factor for a plane wave running in z-direction.

The inelastic contribution to the stress tensor of a fluid has been discussed in Chap. 2, it is

$$T''_{ik} = \eta^{\mathrm{b}}\delta_{ik}\partial_j v_j + \eta^{\mathrm{s}}\left\{\partial_i v_k + \partial_k v_i - \frac{2}{3}\delta_{ik}\partial_j v_j\right\}. \tag{4.408}$$

η^{b} and η^{s} are the bulk and shear viscosity, respectively. The momentum balance equation (2.13), if linearized, reads

$$\bar{\varrho}\delta_t\tilde{v}_i + \partial_i\tilde{p} = \eta^{\mathrm{s}}\Delta\tilde{v}_i + \left\{\frac{\eta^{\mathrm{s}}}{3} + \eta^{\mathrm{b}}\right\}\partial_i\partial_j\tilde{v}_j, \tag{4.409}$$

instead of Eq. (4.386). As before, we work out the divergence and make use of the mass balance equation. One arrives at

$$\left\{\partial_t^2 - \frac{\eta}{\bar{\varrho}}\Delta\,\partial_t\right\}\tilde{\varrho} - \Delta\tilde{p} = 0, \tag{4.410}$$

where $\eta = 4\eta^{\mathrm{s}}/3 + \eta^{\mathrm{b}}$.

We assume that the effect of friction, $\omega\eta/\bar{\varrho}c^2$, is small. Equation (4.410) then may be rewritten as

$$\left\{\frac{1}{c^2}\partial_t^2 - \frac{\eta}{\bar{\varrho}c}\frac{1}{c^3}\partial_t^3 - \Delta\right\}\tilde{p} = 0. \tag{4.411}$$

We insert a plane wave with real angular frequency ω and complex wave number k. The wave equation now becomes an algebraic equation, namely

$$\frac{\omega^2}{c^2} + \mathrm{i}\,\frac{\eta}{\bar{\varrho}c}\,\frac{\omega^3}{c^3} - k^2 = 0, \tag{4.412}$$

the solution of which is

$$k = \frac{\omega}{c} + \mathrm{i}\alpha \text{ where } \alpha = \frac{\eta}{2\bar{\varrho}c}\,\frac{\omega^2}{c^2}. \tag{4.413}$$

The attenuation coefficient α is proportional to the viscosity coefficient and grows quadratically with frequency—a plausible result.

By the way, Eq. (4.413) remains correct if heat conductivity is included [10]. One only has to replace η by

$$\eta = \frac{4}{3}\eta^{\mathrm{s}} + \eta^{\mathrm{b}} + \frac{2}{5}\,\frac{\kappa}{C_{\mathrm{p}}}. \tag{4.414}$$

η^{s} and η^{b} are the shear and bulk viscosities, respectively. The factor 2/5 is specific for a two atomic gas, such as air. κ denotes the heat conduction constant of the gas, and C_{p} is the specific heat capacity at constant pressure.

We here have presented the classical theory of sound attenuation which is based on the assumption that local equilibrium is attained instantaneously. A more detailed study reveals that relaxations should be taken into account. A small part of the molecules is not in its vibrational ground state, but excited, and a perturbation by a pressure wave changes that fraction, until the system relaxes to its equilibrium. The relaxation times for oxygen and nitrogen are different, so that the dependency of the attenuation constant on frequency becomes rather complex. The gross $\alpha \propto \omega^2$ feature however still prevails. For further details see *Springer Handbook of Acoustics* (loc. cit.).

4.22 Stokes' Law

We shall work out the drag of an incompressible viscous fluid on a resting sphere, or the friction encountered when a sphere moves in a resting liquid. We restrict ourselves to laminar flow, a flow without turbulence. The flow velocity must be small, or the viscosity high for Stoke's law to be applicable.

4.22.1 The Problem

Think of a steady flow with constant velocity $v_1 = v_2 = 0$ and $v_3 = v_\infty$. This flow is perturbed by a sphere of radius R fixed at the origin. The boundary conditions hence are

$$\boldsymbol{v}(\boldsymbol{x}) = 0 \text{ for } r = \sqrt{x_1^2 + x_2^2 + x_3^2} = R \tag{4.415}$$

and

$$\boldsymbol{v}(\boldsymbol{x}) = \begin{pmatrix} 0 \\ 0 \\ v_\infty \end{pmatrix} \text{ for } r \to \infty. \tag{4.416}$$

The equation to be solved is Eq. (2.17), the Navier-Stokes equation for a Newtonian incompressible fluid, namely

$$\varrho\{\partial_t v_k + v_i \partial_i v_k\} = -\partial_k p + \eta \Delta v_k. \tag{4.417}$$

If the velocity is very small, or if the viscosity η is very large, then the second term on the right hand side of Eq. (4.417) may be neglected. It is precisely this term which makes the Navier-Stokes equation non-linear with respect to the velocity field and therefore so difficult to solve. More precisely, we demand that the Reynolds number of the problem,

$$\mathtt{Re} = \frac{\varrho v_\infty R}{\eta} \tag{4.418}$$

be much smaller than 1. Since we also look for a steady flow, the time derivative vanishes, and we have to deal with the seemingly simple equations

$$\partial_k p = \eta \Delta v_k \tag{4.419}$$

and

$$\partial_i v_i = 0. \tag{4.420}$$

The latter says that the fluid be incompressible. They describe a creeping or a Stokes flow.

The problem is to find a divergence free velocity field which respects both boundary conditions (4.415) and (4.416). The momentum balance equation—or better, what is left of it—merely serves to determine the pressure.

4.22.2 Vorticity and Stream Function

It is advisable to introduce spherical coordinates r, θ, ϕ by

$$x_1 = r \sin\theta \cos\phi \ , \ x_2 = r \sin\theta \sin\phi \ , \ x_3 = r \cos\theta. \tag{4.421}$$

There are three unit vectors

$$\boldsymbol{n}_r = \begin{pmatrix} \cos\theta \cos\phi \\ \cos\theta \sin\phi \\ \sin\theta \end{pmatrix} , \ \boldsymbol{n}_\theta = \begin{pmatrix} -\sin\theta \cos\phi \\ -\sin\theta \sin\phi \\ \cos\theta \end{pmatrix} , \ \boldsymbol{n}_\phi = \begin{pmatrix} -\sin\theta \sin\phi \\ \sin\theta \cos\phi \\ 0 \end{pmatrix} \tag{4.422}$$

which are orthogonal with each other. The velocity may be expressed as

$$\boldsymbol{v} = v_r \boldsymbol{n}_r + v_\theta \boldsymbol{n}_\theta + v_\phi \boldsymbol{n}_\phi . \tag{4.423}$$

Since the flow far away from the obstacle and the obstacle itself are invariant with respect to rotations about the 3-axis, we assume the same symmetry for the solution. The field v_ϕ vanishes, the components v_r and v_θ depend on r and θ only. This is a considerable simplification. Equation (4.420) now reads

$$\frac{1}{r^2}\partial_r r^2\, v_r + \frac{1}{r\sin\theta}\partial_\theta \sin\theta\, v_\theta = 0. \tag{4.424}$$

The boundary condition (4.415) is

$$v_r(R,\theta) = v_\theta(R,\theta) = 0, \tag{4.425}$$

while Eq. (4.416) says

$$v_r(r,\theta) = v_\infty \sin\theta \text{ and } r_\theta(r,\theta) = v_\infty \cos\theta \text{ for } r \to \infty. \tag{4.426}$$

The procedure to solve Eq. (4.424) with boundary conditions such as Eqs. (4.425) and (4.426) resembles the method which we have explained in the article on *Stress Concentration*. There is a stream function $\Psi = \Psi(r,\theta)$ such that

$$v_r = \frac{1}{r^2\sin\theta}\partial_\theta\Psi \text{ and } v_\theta = -\frac{1}{r\sin\theta}\partial_r\Psi. \tag{4.427}$$

This velocity field is automatically free of divergences. Moreover, the stream function is biharmonic as we shall show next.

Generally, the vorticity of a flow velocity field is defined as

$$\boldsymbol{\omega} = \nabla \times \boldsymbol{v}, \tag{4.428}$$

its divergence vanishes, and for a Stokes flow we find $0 = \nabla \times \nabla p = \eta\Delta\nabla \times \boldsymbol{v}$, i.e.,

$$\nabla \cdot \boldsymbol{\omega} = 0 \text{ and } \Delta\boldsymbol{\omega} = 0. \tag{4.429}$$

Let us now specialize to a two-dimensional flow with $v_x = v_x(x,y)$ and $v_y = v_y(x,y)$. x, y are Cartesian coordinates where the gradient, divergence and curl operators are simple expression. The velocity components are derived from a stream function $\Psi = \Psi(x,y)$ by

$$v_x = \partial_y\Psi \text{ and } v_y = -\partial_x\Psi. \tag{4.430}$$

This velocity field is automatically free of divergences. Its vorticity is calculated to be $\omega_1 = \omega_2 = 0$ and $\omega_3 = -(\partial_x^2 + \partial_y^2)\Psi$. It follows from Eq. (4.429) that the stream function satisfies

$$\Delta\Delta\psi = \left\{\partial_x^4 + 2\partial_x^2\partial_y^2 + \partial_y^4\right\}\Psi = 0. \tag{4.431}$$

If a different coordinate system is used, this equation must be translated. We conclude that the stream function $\Psi = \Psi(r, \theta)$ of Eq. (4.427) is biharmonic.

4.22.3 The Solution

We search for a biharmonic stream function $\Psi = \Psi(r, \theta)$ which gives rise to a velocity field v_r and v_θ according to Eq. (4.427). This velocity field must respect boundary conditions at infinity and at $r = R$. The former refer to a steady flow with velocity v in z-direction, the latter require zero velocity at the obstacle. The solution procedure is very similar to what we have explained in more detail in the article on *Stress Concentration*. We do not repeat it here but simply state the result:

$$\frac{v_k}{v_\infty} = \left(1 - \frac{3}{4}\xi - \frac{1}{4}\xi^3\right)\delta_{3k} + \frac{3}{4}(-\xi + \xi^3)\frac{x_k x_3}{r^2} \text{ where } \xi = \frac{R}{r}. \tag{4.432}$$

With $r \to \infty$ or $\xi \to 0$ the velocity is indeed $v_1 = v_2 = 0$ and $v_3 = v_\infty$. Likewise, for $r = R$ or $\xi = 1$, the velocity $\boldsymbol{v}$ vanishes. If you do not shy away from difficult calculations, check $\nabla \cdot \boldsymbol{v} = 0$.

The velocity field is best visualized by streamlines $\boldsymbol{x}(t)$ which are defined by the differential equation

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{v}(\boldsymbol{x}(t)). \tag{4.433}$$

We have plotted them in Fig. 4.20. Dots on the same streamline represent the position of a material point after fixed time intervals.

4.22.4 Stoke's Formula

The force exerted by the fluid on the sphere is

$$F_i = \int_{|\boldsymbol{x}|=R} \mathrm{d}A_j\, T_{ij}. \tag{4.434}$$

The stress tensor has two contributions, namely

$$T_{ij} = T'_{ij} + T''_{ij} = -p\delta_{ij} + \eta(\partial_i v_j + \partial_j v_i), \tag{4.435}$$

pressure and friction.

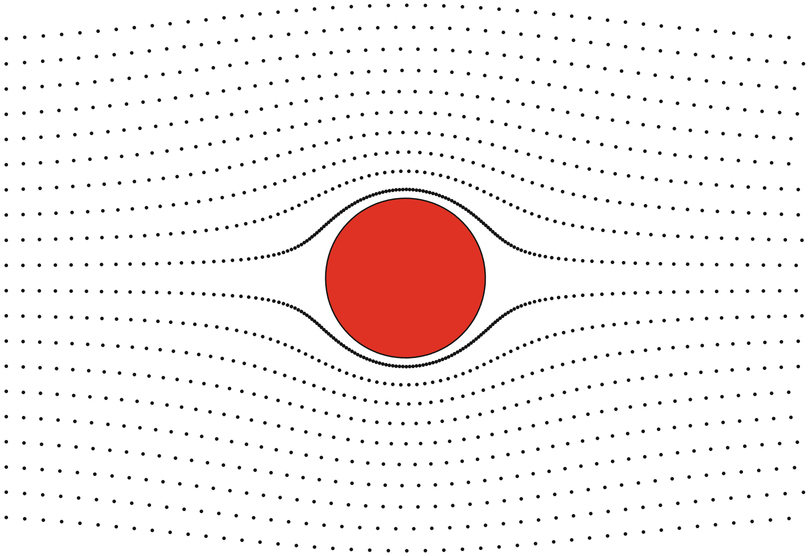

Fig. 4.20 Laminar flow from *left* to *right* around a sphere. The positions z, x of material points are plotted in equal time steps. The separation of points on a stream line is a measure of speed. This figure visualizes the integration of Eq. (4.432) with respect to time

The velocity field is known, hence the pressure gradient $\partial_k p = \eta \Delta v_k$ may be calculated and integrated to

$$p = p_\infty - \frac{3}{2}\frac{R}{r^2}\frac{x_3}{r}\eta v_\infty. \tag{4.436}$$

Its contribution to the force on the sphere is

$$F_3' = 3\pi\eta R v_\infty, \tag{4.437}$$

while $F_1' = F_2' = 0$, as expected. Friction contributes by the same amount, namely

$$F_3'' = 3\pi\eta R v_\infty \tag{4.438}$$

and $F_1'' = F_2'' = 0$. Altogether there is a force on the sphere in stream direction of

$$F = 6\pi\eta R v_\infty. \tag{4.439}$$

This is Stoke's law: the force is proportional to the viscosity η, to the linear dimension R and to the flow speed far away from the obstacle. If the obstacle is a sphere, the geometry factor is 6π.

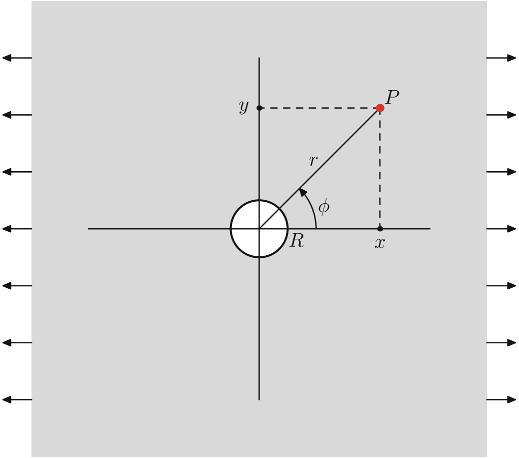

Fig. 4.21 The infinite x, y plane with a circular hole of radius R at the *center*. The plane, far away from the hole, is under uniaxial stress as indicated by the *force arrows*. A material point P is characterized either by Cartesian coordinates (x, y) or by polar coordinates (r, ϕ)

Let us stress once more that Stoke's law (4.439) is valid only for an incompressible Newtonian fluid and for creeping flow.

4.23 Stress Concentration

Imperfections of all kinds may impair the structural properties of devices. In particular, cracks or similar defects will give rise to locally enhanced stress which then may surpass its stability limits. We demonstrate this by calculating the stress distribution in an infinite thin plate under uniaxial stress. At the center, there shall be an imperfection which we model by a circular hole. It turns out that in the vicinity of the hole the stress increases by a factor up to three.

4.23.1 Circular Hole in a Thin Plate

Figure 4.21 explains the notation. We will calculate the stress tensor at an arbitrary point P which may be represented either by Cartesian coordinates x, y or by polar coordinates r, θ for the $z = 0$-plane. They are related by

$$x = r\cos\phi \text{ and } y = r\sin\phi. \tag{4.440}$$

Since the plate is thin, the coordinate z plays no role, we haven a planar problem to solve. One boundary condition to observe is

$$\begin{pmatrix} T_{xx} & T_{xy} \\ T_{yx} & T_{yy} \end{pmatrix} = \begin{pmatrix} \tau_\infty & 0 \\ 0 & 0 \end{pmatrix} \tag{4.441}$$

far away from the hole, i.e., for $\sqrt{x^2 + y^2} = r \to \infty$. The other condition pertains to the hole boundary at $r = R$ which is formulated best in polar coordinates.

The area element for growing distance r from the z-axis is

$$\mathrm{d}A_r = \mathrm{d}r\,\mathrm{d}z \begin{pmatrix} \cos\phi \\ \sin\phi \\ 0 \end{pmatrix}, \tag{4.442}$$

while for growing angle ϕ it is

$$\mathrm{d}A_\phi = r\mathrm{d}\phi\,\mathrm{d}z \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}. \tag{4.443}$$

The forces in r- and ϕ-directions are

$$\mathrm{d}F_r = \mathrm{d}z\left\{T_{rr}\,\mathrm{d}r + T_{r\phi}\,r\mathrm{d}\phi\right\} \tag{4.444}$$

and

$$\mathrm{d}F_\phi = \mathrm{d}z\left\{T_{\phi r}\,\mathrm{d}r + T_{\phi\phi}\,r\mathrm{d}\phi\right\}, \tag{4.445}$$

respectively. The stress tensor with respect to polar coordinates is

$$T_{rr} = \cos^2\phi\,T_{xx} + 2\cos\phi\sin\phi\,T_{xy} + \sin^2\phi\,T_{yy}, \tag{4.446}$$

$$T_{\phi\phi} = \sin^2\phi\,T_{xx} - 2\cos\phi\sin\phi\,T_{xy} + \cos^2\phi\,T_{yy}, \tag{4.447}$$

and

$$T_{r\phi} = -\cos\phi\sin\phi\,T_{xx} + (\cos^2\phi - \sin^2\phi)\,T_{xy} + \cos\phi\sin\phi\,T_{yy}. \tag{4.448}$$

The tensor elements (4.446)–(4.448) are functions of r and ϕ, and the tensor again is symmetric, $T_{r\phi} = T_{\phi r}$.

The boundary condition at the edge of the hole is that the plate does not exert a normal force, $\mathrm{d}F_r = 0$. Therefore,

$$T_{rr}(R,\phi) = T_{r\phi}(R,\phi) = 0 \tag{4.449}$$

must hold true. The condition for static equilibrium—there are no external forces—reads

$$\partial_x T_{xx} + \partial_y T_{xy} = 0 \text{ and } \partial_x T_{yx} + \partial_y T_{yy} = 0. \tag{4.450}$$

4.23.2 Airy's Stress Function for Planar Problems

As emphasized in the section on *Solid Media*, it is not sufficient to solve the equilibrium equations (4.450) for given boundary conditions. The stress tensor must be related with a strain tensor by Hooke's law which, in turn, is to be derived from a displacement field. There are compatibility requirements to be observed. Normally, one can guess the form of the displacement field which may contain yet unknown functions. Deriving the strain and stress tensors yields differential equations for the unknown functions. In our case, there is no obvious guess for the displacement, we have to resort to a potential method.

There is an analogy with the electrostatic field which must be a solution of $\epsilon_0 \nabla \cdot \boldsymbol{E} = \varrho$. However, not every solution is admissible, it must also respect $\nabla \times \boldsymbol{E} = 0$. The latter is guaranteed if the electric field is the gradient of a scalar potential, $\boldsymbol{E} = -\nabla \Phi$. Φ then has to obey $\epsilon_0 \Delta \Phi = \varrho$.

Something similar is known in elasticity theory. The method is particularly simple for planar problems. Assume a sufficiently differentiable Airy stress function $\Phi = \Phi(x, y)$ of two variables. The stress tensor is derived from it by

$$T_{xx} = \partial_y^2 \Phi \;,\; T_{yy} = \partial_x^2 \Phi \text{ and } T_{xy} = T_{yx} = -2 \partial_x \partial_y \Phi. \tag{4.451}$$

We refrain from proving it: any stress tensor defined by Eq. (4.451) satisfies the compatibility requirements. The translation of Eq. (4.451) into polar coordinates reads

$$T_{rr} = \left\{ \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_\phi^2 \right\} \Phi \;,\; T_{\phi\phi} = \partial_r^2 \Phi \text{ and } T_{r\phi} = -\partial_r \frac{1}{r} \partial_\phi \Phi. \tag{4.452}$$

The Airy stress function itself has to obey

$$\Delta \Delta \Phi = \{ \partial_x^4 + 2 \partial_x^2 \partial_y^2 + \partial_y^4 \} \Phi = 0, \tag{4.453}$$

it is biharmonic.[51]

4.23.3 The Solution

The stress tensor at infinity is $T_{xx} = \tau_\infty$, the remaining elements vanishing. We achieve this by

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[51] A harmonic function $f = f(x, y)$ is a solution of $\Delta f = 0$ where $\Delta = \partial_x^2 + \partial_y^2$. A biharmonic function fulfills $\Delta \Delta f = 0$.

$$\Phi = \frac{\tau_\infty}{2} y^2 = \frac{\tau_\infty}{2} r^2 \sin^2\phi = \frac{\tau_\infty}{4} r^2 (1 - \cos 2\phi). \tag{4.454}$$

This Airy stress function is biharmonic, as any polynomial in x and y of degree less than four. We shall try to find Airy stress functions which are compatible with the boundary condition at $r = R$, one axially symmetric, the other one varying as $\cos 2\phi$, and add them as prescribed by Eq. (4.454). Both obey ordinary differential equations.

An axially symmetric Airy stress function $\Phi(r, \phi) = f(r)$ is biharmonic if it fulfills

$$f'''' + \frac{2}{r} f''' - \frac{1}{r^2} f'' + \frac{1}{r^3} f' = 0, \tag{4.455}$$

its general solution is given by

$$f = \tau_\infty R^2 \{a\xi^{-2} \ln \xi + b\xi^{-2} + c \ln \xi + d\} \text{ where } \xi = \frac{R}{r}. \tag{4.456}$$

Comparing with Eq. (4.454) leads to $a = 0$ and $b = 1/4$. d vanishes if stresses are worked out. The remaining constant is fixed by $T_{rr}(R, \phi) = 0$ which results in $c = 1$. Note that $T_{r\phi}$ vanishes identically for an axially symmetric Airy stress function.

Let us now study an Airy stress function $\Phi(r, \phi) = g(r) \cos 2\phi$. It is biharmonic if g obeys

$$g'''' + \frac{2}{r} g''' - \frac{9}{r^2} g'' + \frac{9}{r^3} g' = 0, \tag{4.457}$$

the general solution being

$$g = \tau_\infty R^2 \{a\xi^{-4} + b\xi^{-2} + c + d\xi^2\}. \tag{4.458}$$

This time the boundary condition (4.454) says $a = 0$ and $b = -1/4$. The boundary conditions $R_{rr} = T_{r\phi} = 0$ for $r = R$, or $\xi = 1$, fix the remaining two constants as $c = 1/2$ and $d = -1/4$.

Both Airy stress functions $f(r)$ and $g(r) \cos 2\phi$ guarantee that the force exerted on the edge of the hole vanishes. Both functions grow as $\tau_\infty r^2/4$ at $r \to \infty$, the former without a dependency on ϕ, the latter must be multiplied by a factor $-\cos 2\phi$. Their sum hence solves the problem. From it results the following stress tensor:

$$T_{rr} = \frac{\tau_\infty}{2} \left\{(1 - \xi^2) + (1 - 4\xi^2 + 3\xi^4) \cos 2\phi\right\}, \tag{4.459}$$

$$T_{\phi\phi} = \frac{\tau_\infty}{2} \left\{(1 + \xi^2) - (1 + 3\xi^4) \cos 2\phi\right\}, \tag{4.460}$$

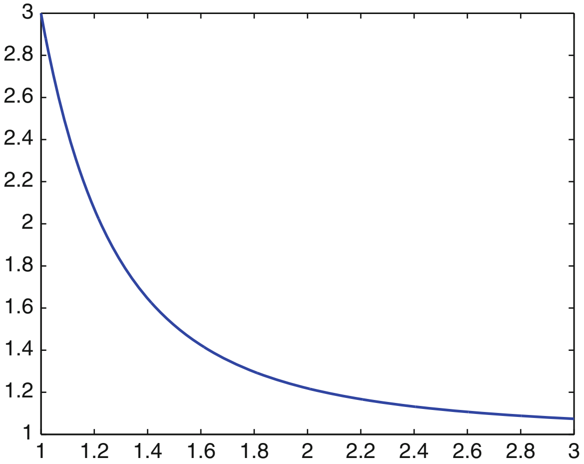

Fig. 4.22 Stress enhancement. Stress T_{xx}/τ_∞ is plotted vs. y/R. See Fig. 4.21 and the text for the meaning of *symbols*. The stress is enhanced by a factor 3 at the hole

and

$$T_{r\phi} = \frac{\tau_\infty}{2}(-1 - 2\xi^2 + 3\xi^4)\ \sin 2\phi. \tag{4.461}$$

4.23.4 Discussion

The solution (4.459)–(4.461) is highly plausible. It falls off rapidly with $r \to \infty$ apart from $T_{rr}(\infty, 0) = T_{\phi\phi}(\infty, \pi/2) = \tau_\infty$. At the edge of the hole, for $r = R$ or $\xi = 1$, both $T_{rr}(R, \phi)$ and $T_{r\phi}(R, \phi)$ vanish. In Fig. 4.22 we have plotted the stress component $T_{\phi\phi}$ vs. y, namely

$$T_{\phi\phi}(r, \frac{\pi}{2}) = T_{\phi\phi}(r, -\frac{\pi}{2}) = T_{xx}(0, y) = \tau_\infty \left\{ 1 + \frac{1}{2}\frac{R^2}{y^2} + \frac{3}{2}\frac{R^4}{y^4} \right\}. \tag{4.462}$$

The stress, the value of which is τ_∞ far away from the hole, is enhanced by a factor up to three in the vicinity of the hole. Note that this factor three does not depend on the radius R of the whole.[52]

This explains why imperfections, such as small holes, are so dangerous. If the device, a reactor vessel for example, can support a certain stress and if there is an imperfection, close to it the stress may exceed the admissible limit. There will be a crack which, being a further origin of stress enhancement, will propagate until the device breaks.

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[52] The limit $R \to 0$ is not allowed because one would leave the realm of continuum physics.

Or think about a line of holes in a sheet of paper (perforation) in order to control where the sheet tears apart.

Already ancient shipbuilders knew that the deck of a boat is an important stabilizing part. There had to be a hole for accommodating the mast. This hole was the preferred spot where, at heavy sea and consequently large stress, the deck ruptured. The edge of the hole in the deck had to be reinforced.

Eyelets in sails or garments are other well known reinforcements to counter stress enhancement by holes.

4.24 Surface Plasmon Polaritons

Light may be guided along a metal's surface. The metal, gold say, is covered by a lossless dielectric medium, for instance air. The permittivity of the metal is a complex number with a large negative real part and, ideally, with a small positive imaginary part. We shall first study a model for the permittivity of a metal in order to make sure that these requirements are realistic. We then show that a light wave is guided by the metal surface.

4.24.1 The Drude Model

Consider the action of an external electric field strength $\boldsymbol{E}$ on a typical electron within a solid. We denote by m its mass, by $-e$ its charge, and by $\boldsymbol{x}$ the deviation from the equilibrium position. The following equation of motion has to be solved:

$$m(\ddot{\boldsymbol{x}} + \varGamma\dot{\boldsymbol{x}} + \varOmega^2\boldsymbol{x}) = -e\,\boldsymbol{E}(t). \tag{4.463}$$

$\varGamma$ describes friction, $m\varOmega^2$ is the spring constant.

We Fourier-transform this equation with respect to time and denote by $\tilde{\boldsymbol{x}}$ and $\tilde{\boldsymbol{E}}$ the Fourier components with respect to angular frequency ω. The time derivative now becomes multiplication with $-\mathrm{i}\omega$, so that Eq. (4.463) reads

$$\tilde{\boldsymbol{x}} = \frac{-e}{m}\frac{1}{-\omega^2 - \mathrm{i}\omega\varGamma + \varOmega^2}\,\tilde{\boldsymbol{E}}. \tag{4.464}$$

The corresponding dipole moment is $-e\tilde{\boldsymbol{x}}$. We denote by N the number of electrons per unit volume. The polarization then is $\tilde{\boldsymbol{P}} = \chi\,\epsilon_0\tilde{\boldsymbol{E}}$ with the susceptibility

$$\chi(\omega) = \frac{Ne^2}{m\epsilon_0}\frac{1}{-\omega^2 - \mathrm{i}\omega\varGamma + \varOmega^2}. \tag{4.465}$$

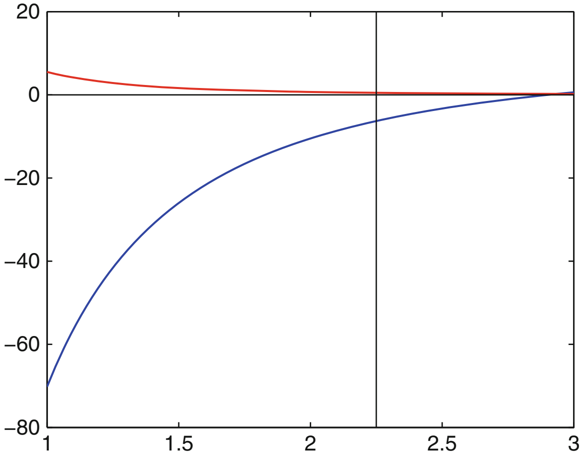

Fig. 4.23 Permittivity of gold according to the free electron gas model. The real part (*lower curve*) and the imaginary part (*upper curve*) are plotted versus photon energy in eV. The model fits experimental data well for photon energies below 2.25 eV (*vertical line*)

The relative permittivity $\epsilon = 1 + \chi$ is

$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_\mathrm{p}^2}{\omega^2 + \mathrm{i}\omega\Gamma} \text{ with } \omega_\mathrm{p}^2 = \frac{Ne^2}{m^*\epsilon_0}. \tag{4.466}$$

There are three modifications which have to be explained. First, we speak of a metal where the electrons in the conduction band form a plasma. Hence, there is no restoring force, $\Omega^2 = 0$. Second, we have written m^* instead of m in the expression for the so called plasma frequency ω_p. The conduction electrons are quasi free particles with an effective mass m^* which will differ from the mass m of free electrons. Third, there are also contributions from bound electrons which arise from much higher frequencies. They will depend only weakly on ω and are included into ϵ_∞. The material equation (4.466) describes the dispersion relation for a gas (plasma) of quasi free electrons, a special case of the original Drude model.

Johnson and Christy have investigated the optical properties of the noble metals [3], among them gold. ϵ_∞ in Eq. (4.466) has the value 9.5. The plasma frequency corresponds to an energy $\hbar\omega_\mathrm{p} = 8.95\,\mathrm{eV}$, friction is characterized by $\hbar\Gamma = 0.069\,\mathrm{eV}$. The corresponding dispersion curve is shown in Fig. 4.23. The free electron gas model fits data well for photon energies below 2.25 eV.

The permittivity of gold is $\epsilon_\mathrm{m} = -6.308 + 0.4848\,\mathrm{i}$ for light of wavelength $\lambda = 0.5513\,\mu\mathrm{m}$ which corresponds to $\hbar\omega = 2.25\,\mathrm{eV}$ (vertical line in Fig. 4.23).

4.24.2 *Guided TM Mode*

We denote by x the coordinate perpendicular to the metal surface. $x > 0$ describes the cover (subscript c), and $x < 0$ the metal (subscript m). Without loss of generality, the direction of propagation on the surface can be chosen as the z axis. All components F of the electromagnetic field $\boldsymbol{E}, \boldsymbol{H}$ are of the form

$$F(t,x,y,z) = F(x)\,\mathrm{e}^{\mathrm{i}\beta z}\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{4.467}$$

ω is the angular frequency of light and β the mode propagation constant.

Maxwell's equations for vanishing charges and currents and for a non-magnetic medium read

$$\nabla \times \boldsymbol{H} = -\mathrm{i}\omega\epsilon_0\epsilon\,\boldsymbol{E} \text{ and } \nabla \times \boldsymbol{E} = \mathrm{i}\omega\mu_0\,\boldsymbol{E}, \tag{4.468}$$

in usual notation. $\epsilon = \epsilon(x)$ is the relative permittivity. Note that both divergence equations are automatically satisfied if $\omega \neq 0$.

A TE mode is specified by

$$\boldsymbol{E} = \begin{pmatrix} 0 \\ E \\ 0 \end{pmatrix} \text{ and } \boldsymbol{H} = \frac{-1}{\omega\mu_0}\begin{pmatrix} \beta E \\ 0 \\ \mathrm{i}E' \end{pmatrix}, \tag{4.469}$$

a TM mode by

$$\boldsymbol{H} = \begin{pmatrix} 0 \\ H \\ 0 \end{pmatrix} \text{ and } \epsilon\,\boldsymbol{E} = \frac{1}{\omega\epsilon_0}\begin{pmatrix} \beta H \\ 0 \\ \mathrm{i}H' \end{pmatrix}. \tag{4.470}$$

For our geometry, $\epsilon\,E_x$ must be continuous as well as E_y, E_z, H_x, H_y, and H_z. In the case of a TE mode, E and E' must be smooth functions. For a TM mode, H and H'/ϵ have to be continuous.

The magnetic field strength obeys the second order differential equation

$$\nabla \times \frac{1}{\epsilon}\nabla \times \boldsymbol{H} = k_0^2\boldsymbol{H}, \tag{4.471}$$

with $\epsilon_0\mu_0c^2 = 1$ and $\omega = k_0c$. For a TM surface mode this boils down to

$$\left\{\epsilon(x)\,\frac{\mathrm{d}}{\mathrm{d}x}\,\frac{1}{\epsilon(x)}\,\frac{\mathrm{d}}{\mathrm{d}x} + k_0^2\,\epsilon(x)\right\}\,H = \beta^2 H. \tag{4.472}$$

For a piecewise constant permittivity profile, Eq. (4.472) simplifies to

$$H'' + k_0^2\,\epsilon(x)\,H = \beta^2 H. \tag{4.473}$$

Let us define[53]

$$\kappa_\mathrm{c} = +\sqrt{\beta^2 - k_0^2\epsilon_\mathrm{c}}. \tag{4.474}$$

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[53] We choose the square root of a complex number such that its real part is positive.

Table 4.5 The TM polarized mode at the surface of gold for light of $\hbar\omega = 2.25\,\mathrm{eV}$. See the text for the meaning of symbols

$\hbar\omega$	2.25	eV
k_0	11.40	$\mu\mathrm{m}^{-1}$
λ	0.5513	$\mu\mathrm{m}$
ϵ_c	1.000	
ϵ_m	$-6.308 + 0.4848\,\mathrm{i}$	
β	$12.42 + 0.08925\,\mathrm{i}$	$\mu\mathrm{m}^{-1}$
κ_c	$4.931 + 0.2247\,\mathrm{i}$	$\mu\mathrm{m}^{-1}$
κ_m	$31.21 - 0.9730\,\mathrm{i}$	$\mu\mathrm{m}^{-1}$
ℓ	5.602	$\mu\mathrm{m}$

Hence, the solution of Eq. (4.473) in the cover region is

$$H(x) = \mathrm{e}^{-\kappa_\mathrm{c} x}, \tag{4.475}$$

which vanishes with $x \to \infty$. We likewise define

$$H(x) = \mathrm{e}^{+\kappa_\mathrm{m} x} \tag{4.476}$$

within the metal, where

$$\kappa_\mathrm{m} = +\sqrt{\beta^2 - k_0^2 \epsilon_\mathrm{m}}. \tag{4.477}$$

With our convention for the square root, Eq. (4.476) will vanish with $x \to -\infty$. Moreover, the magnetic field is already continuous at $x = 0$. In order for $H'(x)/\epsilon(x)$ to be continuous there we require

$$\frac{-\kappa_\mathrm{c}}{\epsilon_\mathrm{c}} = \frac{\kappa_\mathrm{m}}{\epsilon_\mathrm{m}}. \tag{4.478}$$

Squaring this expression yields

$$\beta^2 = k_0^2 \frac{\epsilon_\mathrm{m}\,\epsilon_\mathrm{c}}{\epsilon_\mathrm{m} + \epsilon_\mathrm{c}}. \tag{4.479}$$

An ideal medium would have a large negative real permittivity. Then, β^2 is positive, and an undamped TM mode will propagate at the interface. For a small imaginary contribution to the metal permittivity, a propagation constant β will result with only a small imaginary contribution. The corresponding TM mode will be weakly damped. Note that there is at most one solution to Eq. (4.478). We have listed the waveguide parameters in Table 4.5.

The mode penetrates $1/2\,\mathrm{Re}\,\kappa_\mathrm{m}$ into the metal, that are 16 nm. Figure 4.24 visualizes the TM polarized surface mode. We calculate $\ell = 5.6\,\mu\mathrm{m}$ for the propagation length $\ell = 1/2\,\mathrm{Im}\,\beta$ of the surface mode. This is large if compared with the mode's penetration depth.

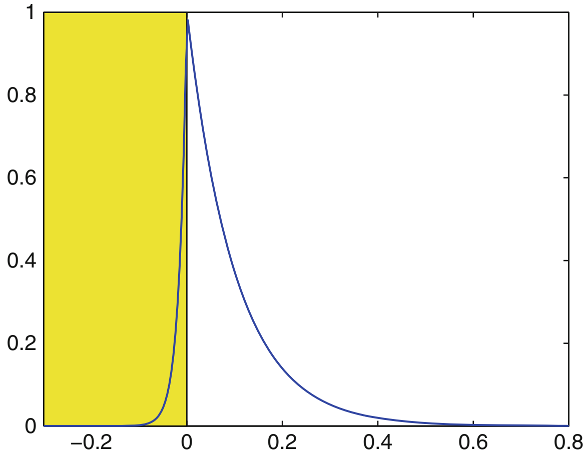

Fig. 4.24 Gold (*shaded*) is covered by air. The intensity profile $|H(x)|^2$ of the TM polarized surface mode is plotted versus the distance (in µm) from the surface. The mode penetrates about 16 nm into the metal. Light wavelength is 0.5513 µm

4.24.3 TE Polarization

For a piecewise constant permittivity the TE mode equation is the same as Eq. (4.473), with H replaced by E. Also the solution is the same. However, this time the field E and its derivative E' must be continuous. Therefore, Eq. (4.478) has to be replaced by

$$-\kappa_{\rm c} = \kappa_{\rm m}. \tag{4.480}$$

Squaring this implies $\epsilon_{\rm c}^2 = \epsilon_{\rm m}^2$, hence $\kappa_{\rm c} = \kappa_{\rm m} = 0$. There is no TE polarized surface mode. This finding holds true for any material on both sides of the interface.

One speaks of surface plasmon polaritons (SPP) because the surface light wave is associated with a plasma polarization wave. Such excitations are quantized, they behave as quasi particles, such as conduction band electrons or holes, phonons, excitons, magnons, solitons, and so forth. Surface plasmon polaritons (SPP) are always TM polarized. SPPs are a subject of current research.

4.25 Thermal Noise of a Resistor

We have derived the dissipation-fluctuation theorem of Callen and Welton in the section on *Fluctuations and Dissipation*. One consequence of it is a proof of the second main law of thermodynamics, at least for linear responses to perturbations of thermodynamic equilibrium. In our article on *Brownian Motion* we independently arrived at Eq. (4.77) which relates a fluctuation of the position of a Brownian particle with its diffusion constant. We shall here discuss thermal noise in electric circuits. Unless a system has been cooled down to zero temperature, its variables fluctuate about the equilibrium value. In particular, we discuss the simplest component of electric circuits, an Ohmic resistor R. We shall see that the resistor produces a

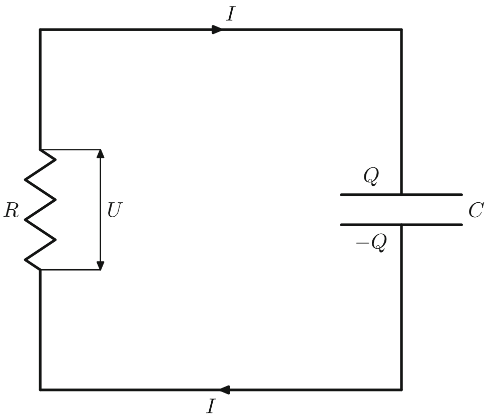

Fig. 4.25 A circuit made up of a resister R and a capacitor C. The charges on the parallel plates are $\pm Q$, respectively. $I = \dot{Q}$ is the current, the voltage across the resister is U

voltage although the circuit of which it is part is completely passive. Its frequency[54] distribution is described by Nyquist's formula. We comment on the role of ensemble averages as used in theoretical considerations and time averages which can be measured.

4.25.1 Langevin Equation

Think of a circuit made up of a resistor R and a parallel plate capacitor C. See Fig. 4.25 for a sketch. There is a charge Q_t on the upper plate and a charge $-Q_t$ on the lower. The electric current in the circuit is $I_t = \dot{Q}_t$. The voltage across the capacitor is $U_t = Q_t/C$. The same voltage is applied to the Ohmic resistor such that current and voltage are related by $U_t = RI_t$. Charge Q_t, current I_t and voltage U_t are time-dependent variables while capacitance C and resistance R are constants. The differential equation

$$RC\dot{U}_t + U_t = 0 \tag{4.481}$$

has the obvious solution

$$U_t = U_0\,\mathrm{e}^{-t/\tau} \text{ where } \tau = RC \tag{4.482}$$

is a time constant. But that is not all.

The free quasi-electrons in a conductor are not entirely free. Otherwise a voltage would accelerate them more and more and there would be an ever increasing current. Instead, the conduction electrons interact with lattice oscillations, or phonons, which brake, or decelerate them. In this way, a constant electric field will drive a stationary electric current.

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[54] We follow electrical engineering tradition and talk of frequencies f instead of angular frequencies $\omega = 2\pi f$.

Now, such interactions will also happen if there is no external electric field. Phonon-electron collisions will spontaneously accelerate conduction electrons, although randomly. There will be, per unit time, as many kicks to the left as to the right, and no net current may develop. However, although a particular conduction electron is not accelerated in the mean, there are random fluctuations. With a small probability many consecutive kicks into the same direction may occur which lead to observable currents and voltages.

We formulate this mathematically by a random electromotive voltage $V = V_t$, such that Eq. (4.481) now reads

$$\tau \dot{U}_t + U_t = V_t. \tag{4.483}$$

The V_t are random variables which are characterized by

$$\langle\, V_t \,\rangle = 0. \tag{4.484}$$

This says that the fanning electromotive voltages are fluctuations, they vanish on the average. Their correlation in time is described by

$$\langle\, V_{t'} V_{t''} \,\rangle = K_V(t' - t''). \tag{4.485}$$

With Eq. (4.485) we take into account that the circuit's parameters do not depend on time. Only time differences count. The Wiener-Khinchin theorem (3.94) with (3.96) says that the time correlation function

$$K_V(t) = \int \mathrm{d}f\, S_V(f)\, \mathrm{e}^{2\pi \mathrm{i} f t} \tag{4.486}$$

is the Fourier transform of a *positive* spectral density function $S_V = S_V(f)$. The latter is defined by

$$\langle\, \tilde{V}^*(f'')\tilde{V}(f') \,\rangle = \delta(f' - f'')S_V(f'). \tag{4.487}$$

Equation (4.483) is a Langevin equation, the random voltage being described by Eqs. (4.484)–(4.486). Its solution depends on initial conditions and the spectral density function $S_V = S_V(f) \geq 0$.

4.25.2 Nyquist Formula

Let us Fourier transform the Langevin equation:

$$-2\pi \mathrm{i} f \tau \tilde{U}_f + \tilde{U}_f = \tilde{V}_f, \tag{4.488}$$

which results in

$$\tilde{U}_f = \frac{\tilde{V}_f}{1 - 2\pi \mathrm{i} f \tau}. \tag{4.489}$$

We conclude that the spectral density of the process $t \to U_t$ is

$$S_U(f) = \frac{S_V(f)}{1 + 4\pi^2 f^2 \tau^2}, \tag{4.490}$$

see Eq. (4.487).

We now assume that random electromotive voltages are correlated only for an extremely short time[55] as compared with the time constant τ of the circuit:

$$K_V(t) = \kappa\, \delta(t) \text{ or } S_V(f) = \kappa \text{ with } \kappa > 0. \tag{4.491}$$

This behavior is called *white noise*. Noise, because the signal $t \to \langle V_t \rangle$ vanishes. White, because the spectral density in the frequency region of interest is constant. This terminology comes from optics where white light is characterized by a constant spectral density within the frequency range of visible light.

For white noise the time correlation function $K_U(t)$ is

$$K_U(t) = \int \mathrm{d}f \, \frac{\kappa}{1 + 4\pi^2 \tau^2 f^2} \, \mathrm{e}^{2\pi \mathrm{i} f t} = \frac{\kappa}{2\tau} \, \mathrm{e}^{-|t|/\tau}. \tag{4.492}$$

As is well-known, the field energy stored in a capacitor is $W = UQ/2 = CU^2/2$ which is equal to $k_\mathrm{B}T/2$ in thermal equilibrium. Because of $K_U(0) = \langle U^2 \rangle$ we calculate

$$k_\mathrm{B}T = C \langle U^2 \rangle = C K_U(0) = C \frac{\kappa}{2\tau} = \frac{\kappa}{2R} \tag{4.493}$$

or

$$S_U(f) = 2Rk_\mathrm{B}T. \tag{4.494}$$

$S_U(f)$, as it appears in the Wiener-Khinchin theorem (4.486), is the power per unit frequency interval. Because, for a *positive* frequency f, the interval $[f, f + \mathrm{d}f]$ and $[-f - \mathrm{d}f, -f]$ are equivalent, we must write

$$\bar{S}_U(f) = S_U(f) + S_U(-f) = 4Rk_\mathrm{B}T. \tag{4.495}$$

This is the famous Nyquist formula for Johnson noise. J.B. Johnson discovered this form of noise in 1927 and published rather accurate measurements in 1928. H. Nyquist, an electrical engineer of Swedish roots who emigrated to the USA, explained it shortly afterwards. Johnson noise is caused by the interactions

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[55] Electronics is limited by µm dimensions, therefore times below $\approx 10^{-14}$ s cannot be resolved. The natural time for phonon-electron interactions is the natural atomic time unit of $\approx 10^{-17}$ s.

between conduction electrons and thermally induced photons, or lattice vibrations. Its spectral density $\bar{S}_U(f)$ does not depend on frequency, at least up to many GHz. Its dependency on T is obvious: higher temperature, more phonons, more interactions. The dependency on R is as well simply to explain: the noise of resistors in series adds up. And: fluctuations in the equilibrium state are always proportional to the Boltzmann constant k_B.

4.25.3 Remarks

Note that the capacitance C does not show up in Nyquist's formula. We could have analyzed a circuit made up of a resistor and an inductor as well. Then the inductivity L would have dropped out. In fact, any circuit of arbitrary impedance Z will serve. The decisive arguments is the equipartition theorem. If the Hamiltonian of a system is a sum of independent observables squared, then each such degree of freedom has an energy $k_BT/2$ in thermal equilibrium. This result of classical statistical mechanics, however, is true only for large enough temperatures. In our case, hf should be small if compared with k_BT. For $T = 300\,\mathrm{K}$ this amounts to $f \ll 6\,\mathrm{THz}$. For higher frequency Nyquist's formula must be corrected by factor which depends on $x = hf/k_BT$ the limit $x \to 0$ of which is 1. For details see the section on *Fluctuations and Dissipation*.

Electronic circuits suffer from many sources of noise. Johnson noise produced by Ohmic resistors is just one of them. Any electric current, which is a stream of charged particles, causes fluctuations because charge is quantized. Such shot noise was discovered by W. Schottky in 1918. It is particular important if only few (n) electrons pass a barrier in a short time. Then the current density fluctuation, which is proportional to $\sqrt{n}$, cannot be ignored.

Another remark seems to be appropriate. No measuring device can measure a signal instantaneously. Neither the human eye nor an electronic device may correlate an event with a precise time, there is always a certain time resolution which imposes a limit on the accuracy. In particular electronic devices always measure a time average which can be adjusted. In fact, measured values of a signal $t \to A_t$ are always time averages, for instance with constant weight:

$$\mathrm{TAV}(A_t) = \frac{1}{2\tau} \int_{t-\tau}^{t+\tau} \mathrm{d}s\, A_s. \tag{4.496}$$

The expectation value $\langle A_t \rangle$ is something else. One has to set up an array of N identical systems, start the same process A at time $t = 0$ in each system and measure $(A_t)_n$ at time t for system $n = 1, 2, \dots N$. The ensemble average is

$$\mathrm{EAV}(A_t) = \frac{1}{N} \sum_{n=1}^{N} (A_t)_n, \tag{4.497}$$

its limit $N \to \infty$ is the expectation value $\langle A_t \rangle$. The latter is the object of theoretical reasoning.

The ergodicity hypothesis states that time averages and ensemble averages coincide for long enough averaging times τ in almost all cases. We just mention this here because the Nyquist formula must be interpreted differently when justified theoretically and checked experimentally. We shall not dwell on this point any more because it is basic to science, in particular physics. How to translate mathematical equations into prescriptions for verifying them experimentally? Or the other side of the same coin: How to map empirical rules into relations between mathematical objects which can be checked for logical truth?

4.26 Thomson, Seebeck and Peltier Effect

In this article on transport we will discuss cross effects: there is more than one generalized force driving more than one generalized flux. To be specific, we want to investigate solid electrical conductors which are good heat conductors as well. Let us see why and how heat and charge conduction are intermingled.

4.26.1 *Solid Conductors*

There is no mass flow, and there are no chemical reactions. Free quasi-electrons are the only species of mobile charged particles, we index them by an asterisk superscript. Recall that electric charge transport ($\boldsymbol{j}^{\mathrm{e}}$) is by convection ($\varrho^{\mathrm{e}}\boldsymbol{v}$) or conduction ($\boldsymbol{J}^{\mathrm{e}}$), the latter being reversible ($\boldsymbol{J}^{\mathrm{e}\prime}$) or irreversible ($\boldsymbol{J}^{\mathrm{e}\prime\prime}$). The reversible part coincides with the time derivative of the polarization which is of no interest here. The irreversible part corresponds to the motion, by drift or diffusion, of free electrons, $\boldsymbol{J}^{\mathrm{f}}$. In this context we may write the electric current density as

$$\boldsymbol{J}^{\mathrm{e}} = -e\boldsymbol{J}^{*}. \tag{4.498}$$

There is a current density $\boldsymbol{J}^{*}$ of electrons each carrying its charge $-e$. However, electrons will transport not only charge, but also internal energy.

Phonons, the quanta of lattice vibrations, are also mobile quasi-particles, they transport internal energy. Phonon diffusion, or heat conduction in this context, is described by the associated heat current $\boldsymbol{J}^{\mathrm{u}}$.

There are two species of mobile particles, phonons and electrons, and two corresponding currents, namely $\boldsymbol{J}^{\mathrm{u}}$ and $\boldsymbol{J}^{\mathrm{e}}$. There are also two driving forces, namely ∇T and $\nabla\psi$, the gradients of temperature T and of the electrochemical potential

$$\psi = \phi^{\mathrm{e}} - \frac{\mu^{*}}{e}. \tag{4.499}$$

4.26.2 Charge and Heat Transport

Let us recall the expression

$$\pi(S) = \boldsymbol{J}^{\mathrm{u}} \cdot \nabla \frac{1}{T} + \boldsymbol{J}^{*} \cdot \nabla \frac{\mu^{*}}{T} + \frac{1}{T} \boldsymbol{J}^{\mathrm{e}} \cdot \boldsymbol{E} \tag{4.500}$$

for the amount of entropy produced per unit volume per unit time. The entropy conduction current is given by

$$\boldsymbol{J}^{\mathrm{s}} = \frac{1}{T} \left(\boldsymbol{J}^{\mathrm{u}} + \frac{\mu^{*}}{e} \boldsymbol{J}^{\mathrm{e}} \right). \tag{4.501}$$

It is a simple exercise to rewrite Eq. (4.500) into

$$\pi(S) = -\frac{1}{T} \left(\boldsymbol{J}^{\mathrm{s}} \cdot \nabla T + \boldsymbol{J}^{\mathrm{e}} \cdot \nabla \psi \right). \tag{4.502}$$

This sum of “flux times force” terms suggests the following linear relationship

$$\begin{pmatrix} \boldsymbol{J}^{\mathrm{s}} \\ \boldsymbol{J}^{\mathrm{e}} \end{pmatrix} = - \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} \nabla T \\ \nabla \psi \end{pmatrix}. \tag{4.503}$$

We have already taken into account Onsager’s relation by postulating a symmetric matrix of kinetic coefficients. This matrix must also be positive which amounts to $A \ge 0$, $C \ge 0$, and $AC \ge B^2$. By comparing

$$\boldsymbol{J}^{\mathrm{e}} = -\sigma (\nabla \psi + \alpha \nabla T) \tag{4.504}$$

with Eq. (4.503) we recognize $\sigma = C$, therefore the electric conductivity σ is always positive. The sign of $\alpha = B/C$ cannot be predicted from first principles. If the temperature is the same everywhere, Eq. (4.504) coincides with Ohm’s law (2.86). Moreover, the chemical potential, which depends on composition and temperature, cannot have a gradient within a homogeneous material, and we may write $\boldsymbol{J}^{\mathrm{e}} = -\sigma \boldsymbol{E}$. Equation (4.504) is a generalization of Ohm’s law, it allows for a temperature gradient which will also drive a charge current.

The second relation contained in Eq. (4.503) may be expressed as

$$\boldsymbol{J}^{\mathrm{u}} = -\lambda \nabla T + \gamma \boldsymbol{J}^{\mathrm{e}} \tag{4.505}$$

where $\lambda = T(A - B^2/C)$ is the heat conductivity. It is guaranteed to be positive. The coefficients γ in Eq. (4.505) and α in Eq. (4.504) are related by

$$\gamma = T\alpha - \frac{\mu^{*}}{e}. \tag{4.506}$$

Without electric current we obtain Fourier's law $\boldsymbol{J}^{\mathrm{u}} = -\lambda\nabla T$. An additional electric current causes additional heat transport. However, the sign of γ (just as the sign of α) cannot be predicted from first principles.

4.26.3 Thomson Effect

Let us work out the heating of a particular material point. We have to calculate

$$\partial_t \varrho u = -\nabla \cdot \boldsymbol{J}^{\mathrm{u}} + \boldsymbol{J}^{\mathrm{e}} \cdot \boldsymbol{E}. \tag{4.507}$$

This expression takes into account that there is no difference between ordinary and substantial time derivative and that only Joule's heat $\boldsymbol{J}^{\mathrm{e}} \cdot \boldsymbol{E}$ contributes to the production of internal energy. By solving Eq. (4.504) for the electrical field strength we arrive at

$$\boldsymbol{E} = \frac{\boldsymbol{J}^{\mathrm{e}}}{\sigma} + \alpha\nabla T - \nabla \frac{\mu^*}{e}. \tag{4.508}$$

This is to be multiplied by $\boldsymbol{J}^{\mathrm{e}}$. On the other hand, because of $\nabla \cdot \boldsymbol{J}^{\mathrm{e}} = 0$, we obtain

$$-\nabla \cdot \boldsymbol{J}^{\mathrm{u}} = \nabla \cdot \lambda\nabla T - \boldsymbol{J}^{\mathrm{e}}\nabla\gamma. \tag{4.509}$$

We refer to Eq. (4.506) and conclude

$$\partial_t \varrho u = \nabla \cdot \lambda\nabla T + \frac{\boldsymbol{J}^{\mathrm{e}} \cdot \boldsymbol{J}^{\mathrm{e}}}{\sigma} - \boldsymbol{J}^{\mathrm{e}} \cdot T\nabla\alpha. \tag{4.510}$$

The first term describes the net inflow of internal energy as caused by a temperature gradient. The second contribution is the rate of internal energy production per unit volume if an electric current flows in a conducting medium, it is always positive.[56] The third term describes the Thomson effect. In a homogeneous material it takes the form $\mu\, \boldsymbol{J}^{\mathrm{e}} \cdot \nabla T$ where the Thomson coefficient is given by

$$\mu = -T\frac{\partial\alpha}{\partial T}. \tag{4.511}$$

This contribution to the heating of a material point is proportional to the electric current and to the temperature gradient. It changes sign if the direction of the electric current is reversed.

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[56] It vanishes in a super-conductor where $1/\sigma = 0$.

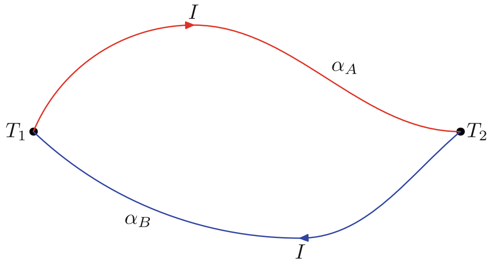

Fig. 4.26 Two wires of different materials A and B are soldered to a circuit. One soldering contact is kept at temperature T_1, the other at T_2. The electric current I flows in the indicated direction if $\alpha_A > \alpha_B$ and $T_2 > T_1$

4.26.4 Seebeck and Peltier Effect

So far we have always assumed that the medium under investigation is spatially homogeneous. We now mention two related effects which show up if different conducting or semi-conducting materials are involved.

Imagine a simple circuit made up of two homogeneous wires of different composition A and B soldered at points P_1 and P_2. These soldering contacts are kept at temperatures T_1 and T_2, respectively. See Fig. 4.26 for a sketch. If the circuit is open, so that no electric current can flow, Eq. (4.504) reads $-\nabla\psi = \alpha\nabla T$. The line integral around the circuit is the electromotive force U,

$$U = -\oint \mathrm{d}\boldsymbol{s}\,\nabla\psi = \oint \mathrm{d}\boldsymbol{s}\,\alpha\nabla T = \int_{T_1}^{T_2} \mathrm{d}T\,(\alpha_A - \alpha_B). \tag{4.512}$$

The circuit is assumed to run from point P_1 via wire A to point P_2 and back via wire B to point P_1. This thermoelectric electromotive force requires different materials and different temperatures at the soldering contacts. If the circuit is electrically closed by an external load, it will drive a current

$$I = \frac{U}{R_\mathrm{i} + R_\mathrm{e}}, \tag{4.513}$$

where R_i and R_e denote the internal and the external resistance, respectively.

The existence of an electromotive force (4.512) caused by soldering different conductors is known as the Seebeck effect. Ironically, Seebeck himself detected the magnetic field associated with Eq. (4.513). He never spotted it down to a current caused by an electromotive force. The Seebeck effect may serve for the direct heat to power conversion. It is, however, rather inefficient. With today's materials the degree of efficiency is much below the Carnot limit $(T_2 - T_1)/T_2$ where T_2 is the higher temperature. Best results are obtained with p-n-semiconductor couples.

The Peltier effect is related to the Seebeck effect. If an electric current $\boldsymbol{J}^{\mathrm{e}}$ flows through a thermocouple, heat is delivered to or subtracted from the soldering contact, depending on the direction of the electric current.

Consider the interface between two different conducting materials A and B. Assume the temperature to be constant on both sides. The normal component of the electric current must be continuous as well as the electric and the electrochemical potential. We conclude that the coefficient γ of Eq. (4.505) jumps by

$$\Pi = T(\alpha_A - \alpha_B) \tag{4.514}$$

at the interface between material A and B. Therefore, the heat current jumps by

$$\boldsymbol{J}^{\mathrm{u}}_{\mathrm{B}} - \boldsymbol{J}^{\mathrm{u}}_{\mathrm{A}} = \Pi \boldsymbol{J}^{\mathrm{e}}. \tag{4.515}$$

This heat current difference is maintained by the heat reservoir to which the interface is coupled. Π is the Peltier coefficient which depends on temperature and on the composition of the two materials soldered together. The Peltier effect allows to heat or cool a soldering contact as desired by controlling an electric current. However, Peltier refrigerators are rather inefficient.

4.27 Vibrating Strings and Membranes

We did not touch the subject in the theory part. Elasticity theory there was concerned with elastic media in three dimensional space. However, there are one- and two-dimensional idealizations, strings and membranes. In both cases we speak of tension: force and force per length, respectively. Likewise μ denotes the mass per unit length of a string or the mass per unit area of a membrane.

4.27.1 Strings

Assume a thin string under tension τ. The string is a straight line with constant small cross section which we parameterize by x. A particular material point at x is drawn at from both sides. The string $y > x$ draws at the material point with a force $\tau(x)$, the string $y < x$ with $-\tau(x)$. The force on an interval $x \le y \le x + \mathrm{d}x$ then is $\tau(x + \mathrm{d}x) - \tau(x) = \tau'(x)\mathrm{d}x$. The unperturbed string shall be at rest, hence the tension τ does not depend on x, it is a constant with the physical dimension of a force.

We now assume that the string is displaced in z-direction by $u = u(x)$. The curve

$$\boldsymbol{\xi}(x) = \begin{pmatrix} x \\ 0 \\ u(x) \end{pmatrix} \tag{4.516}$$

has a tangent vector

$$\frac{\mathrm{d}\boldsymbol{\xi}(x)}{\mathrm{d}x} = \boldsymbol{t}(x) = \begin{pmatrix} 1 \\ 0 \\ u'(x) \end{pmatrix} \tag{4.517}$$

the length of which is

$$|\boldsymbol{t}(x)| = \sqrt{1 + u'(x)^2}. \tag{4.518}$$

The force exercised by the string to the left of x is

$$\boldsymbol{F}(x) = -\tau \frac{1}{\sqrt{1 + u'(x)^2}} \begin{pmatrix} 1 \\ 0 \\ u'(x) \end{pmatrix}, \tag{4.519}$$

while the string right to $x + \mathrm{d}x$ draws with

$$\boldsymbol{F}(x + \mathrm{d}x) = +\tau \frac{1}{\sqrt{1 + u'(x + \mathrm{d}x)^2}} \begin{pmatrix} 1 \\ 0 \\ u'(x + \mathrm{d}x) \end{pmatrix}. \tag{4.520}$$

We assume that the displacement gradient is small, $|u'(x)| \ll 1$. Then the sum of the two forces (4.519) and (4.520) has no x-component, and the z-component is

$$\mathrm{d}F(x) = \tau\, \mathrm{d}x\, u''(x). \tag{4.521}$$

This force is balanced by the product of mass times acceleration. With μ as mass per unit string length we write

$$\left\{ \frac{1}{c^2} \partial_t^2 - \partial_x^2 \right\} u = 0 \text{ where } c = \sqrt{\frac{\tau}{\mu}}. \tag{4.522}$$

This is a one-dimensional wave equation, the sound velocity being c.

4.27.2 Membranes

Consider a region Ω in the x, y plane. It shall be covered by a thin membrane under constant tension τ. Tension in the context of a tow-dimensional manifold is a force per unit length. Likewise, we speak of a mass μ per unit area. More generally, tension should be described by a symmetric tensor τ in two dimensions. τ_{xx} may differ from τ_{yy}. Just think of a thin rubber band which is stretched much in x-direction and less in y-direction. Here we concentrate on a fluid-like tension, a situation without shear, where the tension is proportional to the unit tensor. Let us displace the membrane in z-direction by $u = u(x, y)$. A membrane element $[x, x + \mathrm{d}x] \times [y, y + \mathrm{d}y]$ suffers four forces each of which has a z-component because the tangential planes of the surface

$$\boldsymbol{\xi}(x, y) = \begin{pmatrix} x \\ y \\ u(x, y) \end{pmatrix} \tag{4.523}$$

are inclined. There is one force proportional to $\mathrm{d}y$ at x, another one proportional to $\mathrm{d}x$ at y, a third proportional to $\mathrm{d}y$ at $x + \mathrm{d}x$, and a fourth proportional to $\mathrm{d}x$ at $y + \mathrm{d}y$.

We assume a small displacement gradient, $|\partial u/\partial_x| \ll 1$ and $|\partial u/\partial_y| \ll 1$. The x- and the y-components of the total force add up to zero, while the z-component is

$$\mathrm{d}F(x, y) = \tau \,\mathrm{d}x\,\mathrm{d}y \left\{ \frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} \right\}. \tag{4.524}$$

This force is compensated by a term of type mass times acceleration:

$$\mu \,\mathrm{d}x\,\mathrm{d}y\, \ddot{u} = \mathrm{d}F, \tag{4.525}$$

which boils down to a wave equation for the time-dependent displacement $u = u(t, x, y)$. In fact, we arrive at

$$\left\{ \frac{1}{c^2}\partial_t^2 - \partial_x^2 - \partial_y^2 \right\} u = 0 \text{ where } c = \sqrt{\frac{\tau}{\mu}}. \tag{4.526}$$

Note the physical dimensions. τ is measured in Newton per meter, and μ in kilogram per square meter, hence c is a velocity. For the vibrating string, τ was measured in Newton and μ in kg per meter, so the symbol c in Eq. (4.523) is a velocity as well.

4.27.3 String Eigenmodes

Think about a string of length ℓ such that $u(0) = u(\ell) = 0$. In order to be concrete, we refer to a violin string which is tuned to the standard pitch of $\omega/2\pi = f = 440\,\mathrm{Hz}$. The four strings of a violin can individually be stressed such that the required tension τ results which gives rise to a desired sound velocity c.

The eigenmodes are solutions of the wave equation which oscillate harmonically:

$$u(t, x) = u(x) \sin \omega t. \tag{4.527}$$

The function $u = u(x)$ has to obey

$$-u'' = \frac{\omega^2}{c^2} u \text{ with } u(0) = u(\ell) = 0. \tag{4.528}$$

This is a typical eigenvalue problem.

For square-integrable complex-valued functions f, g we may define the following scalar product:

$$(g, f) = \frac{1}{\ell} \int_0^\ell \mathrm{d}x\, g^*(x)\, f(x). \tag{4.529}$$

The operator ∂_x^2 on the left hand side of Eq. (4.529) with its boundary conditions[57] is self-adjoint,

$$(g, f'') = (g'', f). \tag{4.530}$$

It follows that the system of eigensolutions is complete.

The eigensolutions of Eq. (4.528) obviously are

$$u_n(x) = \sqrt{2} \sin \frac{n\pi x}{\ell} \text{ for } n = 1, 2, \ldots. \tag{4.531}$$

They form a complete set of normalized, mutually orthogonal functions:

- They are normalized, $(u_n, u_n) = 1$,
- Different eigenfunctions are orthogonal, $(u_m, u_n) = 0$ for $m \neq n$,
- They are complete so that any reasonable function may be written as a superposition of eigenfunctions.

The latter statement says that, for any square integrable function $f = f(x)$, the sequence

$$f_N(x) = \sum_{n=1}^{N} (u_n, f)\, u_n(x) \tag{4.532}$$

converges towards f in the sense of

$$\lim_{N\to\infty} \frac{1}{\ell} \int_0^\ell \mathrm{d}x\, |f(x) - f_N(x)|^2 = 0. \tag{4.533}$$

Please note that the function f must not vanish at $x = 0$ or $x = \ell$ although all f_N do so. $f_N \to f$ in general does not converge point-wise. Likewise, f must not be differentiable although each f_N is infinitely often differentiable. Figure 4.27 depicts an example.

Figure 4.27 may serve as a crude example for how a string is excited. On a guitar, or on a piano, the string is hit at a certain place, usually somewhere around the middle. This produces a triangle function like displacement which is made up of the fundamental tone and a series of overtones, or harmonics, with definite phases.

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[57] ∂_x^2 is defined for twice differentiable functions vanishing at $x = 0$ and $x = \ell$.

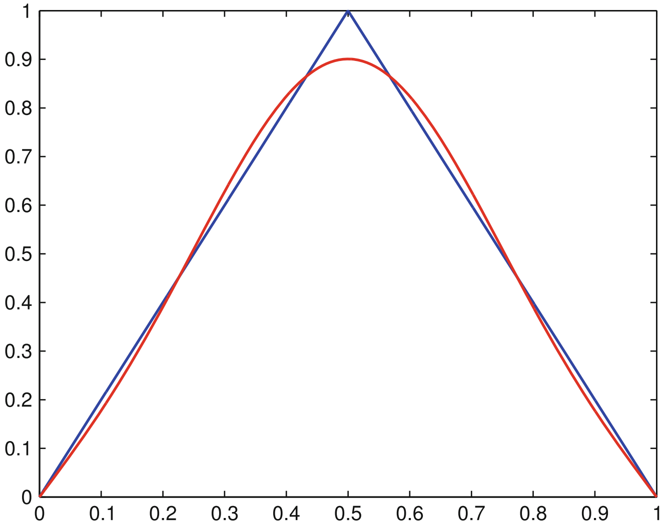

Fig. 4.27 The triangle function on $0 \leq x \leq 1$ and its representation by only three terms of the expansion into eigenfunctions. The discrepancy is largest where the function is not differentiable

This superposition of vibrations is coupled into the musical instrument which in turn produces more vibrations with different frequencies.

A string of length ℓ with tension τ and mass μ per unit length produces a fundamental tone with angular frequency

$$\omega_1 = \frac{\pi c}{\ell} \text{ with } c = \sqrt{\frac{\tau}{\mu}}. \tag{4.534}$$

The basic tone and its overtones are characterized by

$$\omega_n = n\omega_1 \text{ for } n = 1, 2, \ldots. \tag{4.535}$$

With a guitar or a violin, a player may determine the effective length ℓ^* of a string. The frequency then changes as ℓ/ℓ^*. Particular frequency ratios are perceived as specially harmonious, like 2:1 (octave), 3:2 (perfect fifth[58]) or 4:3 (perfect fourth), and so on. The sensory concordance of a perfect fifth and a few more intervals can easily be understood: the third octave of the lower tone and the second octave of the higher are the same. Probably for this reason, the four strings of the violin family of musical instruments are tuned in perfect fifths. When tuning the instrument, the player increases or decreases tension until the interval to the adjacent string is a perfect fifth which produces a particularly pleasant sound.

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[58] Also quint, Quinte (German), quinta (Italian).

There are very many musical scales most of which repeat after one octave. Most common in western music are the diatonic major and minor scales. C major is made up of C-D-E-F-G-A-B-C, where the steps E-F and B-C are half tones, the remaining are whole tones.[59] A-minor is the scale A-B-C-D-E-F-G-A. Again the half tone steps are B-C and E-F, but in a different order as compared with the major scale.

In just (or pure) intonation the frequency ratios are rational numbers with small nominators and denominators. They are D:C=9:8, E:C=5:4, F:C=4:3, G:C=3:2, A:C=5:3 and B:C=15:8. This one is good for a piece of music in C-major or A-minor. However, if the same ratios are to be valid for a work in D-major, for example, then E:D should be 9:8, but it is (5/4):(9/8)=10:9. Thus, apart from the violin family, all instruments had to be exchanged or re-tuned, if possible.

During Bach's lifetime a new tuning scheme for keyboard instruments and harpsichords came into use. A scale consists of five whole tone and two half tone intervals, altogether twelve half tones. If the half tone ratio is fixed, namely

$$R = \sqrt[12]{2} = 1.0594631\ldots, \tag{4.536}$$

then a whole tone interval is just two half tone intervals, and each tone has a fixed frequency irrespective of the musical scale. Raising a tone by a half tone or lowering the next whole tone by a half tone is the same, as expressed by D♭=C♯ and so on. This tuning scheme, the chromatic scale, was called "well tempered".

However, there is a price to pay. For example, the perfect fifth of a scale is described by the ratio 3:2. In the well tempered tuning it is $R^7 = 1.498$. The discrepancy of 0.13% can be perceived by the human ear (and brain), in principle. However, keyboard instruments or harpsichords produce tones of rather short duration $\delta\tau$. Consequently, not one frequency f is excited, but many, and their spread δf is given by $\delta\tau\,\delta f \approx 1$. With $\delta\tau = 1$ s the frequency spread is 1 Hz. 0.13% of 440 Hz is 0.6 Hz, so the discrepancy is tolerable.

The well-tempered clavier[60] by Johann Sebastian Bach comes in two volumes of 24 pieces each. For all tones of the chromatic scale there is a major part and a minor part: C major, C minor, C♯ major, C♯ minor, …, B major and B minor. All these preludes and fugues could be played on one and the same instrument without re-tuning ! Bach himself regarded *Das wohltemperierte Clavier* as central to his work, and many of his admirers look at it as central to western classical music in general.

There is much more to say on vibrating strings and music, but we have to stop here.

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[59] In German nomenclature B is denoted as H and H♭ as B; cf. the well-known B-A-C-H motif.

[60] *Das wohltemperierte Clavier* in German. *Clavier* in this context is any keyboard instrument, not just the piano or Klavier in German. The first volume was completed in 1722, the second in 1742.

4.27.4 Membrane Eigenmodes

As explained above, a vibrating membrane is described by the wave equation (4.526). The displacement $z = u(t, x, y)$ is to be calculated within a region Ω subject to the boundary condition $u(t, x, y) = 0$ on $(x, y) \in \partial\Omega$, the boundary.

We look for eigenmodes which oscillate harmonically in time,

$$u(t, x, y) = u(x, y)\, \sin \omega t. \tag{4.537}$$

The function $u = u(x, y)$ has to obey

$$\left\{ -\partial_x^2 - \partial_y^2 \right\} u = \frac{\omega^2}{c^2} u \text{ and } u(x, y) = 0 \text{ on } (x, y) \in \partial\Omega. \tag{4.538}$$

This is a standard eigenvalue problem.

We define the scalar product for two functions living on Ω as

$$(g, f) = \frac{1}{\text{area}(\Omega)} \int_{\Omega} \mathrm{d}x\mathrm{d}y\, g^*(x, y) f(x, y). \tag{4.539}$$

With it, the two-dimensional Laplacian $\partial_x^2 + \partial_y^2$ is self-adjoint, and the set of eigensolutions of Eq. (4.536) is complete.

As an example, consider the rectangle $\Omega = [0, a] \times [0, b]$. Its eigenfunctions factorize, they are

$$u_{mn} = 2 \sin \frac{m\pi x}{a} \sin \frac{n\pi y}{b} \text{ for } m = 1, 2, \dots \text{ and } n = 1, 2, \dots. \tag{4.540}$$

They form a complete orthonormal set:

$$(u_{rs}, u_{mn}) = \delta_{rm} \delta_{sn}, \tag{4.541}$$

and any square integrable function $u = u(x, y)$ on Ω can be written as

$$u(x, y) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} (u_{mn}, u)\, u_{mn}(x, y). \tag{4.542}$$

Figure 4.28 visualizes the mode u_{32} on a square region as a contour plot.

There is also an exact solution for a circular disk which models a drum. However, apart from such highly symmetric situations, the eigenvalue problem has to be solved numerically. Standard methods are the finite difference method FDM and the finite element method FEM.

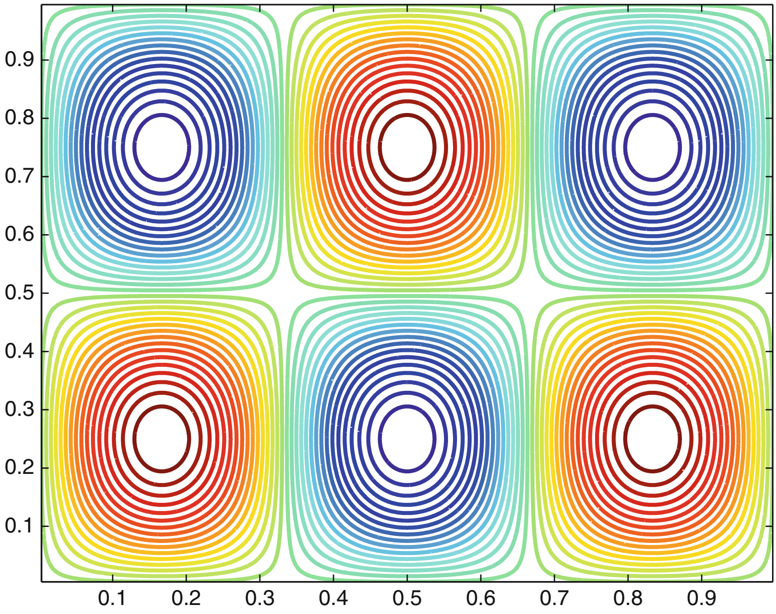

Fig. 4.28 The eigenmode u_{32} of a rectangular membrane. The *contour lines* correspond to equal displacement $z = u(x, y)$. Adjacent vibrations oscillate with opposite phase: *upper left upwards, lower left* and *upper second downwards*, and so on

This is not the place to elaborate on numerical methods for solving partial differential equations, however, a few remarks seem to be appropriate. The finite difference method and the finite element method have in common that they represent the region Ω by representative points and the field u by values at these points which are variables. The finite difference method in its simplest form relies on equal spacing. (x, y) is represented by (ih, jh) where h is the mesh spacing and i, j are integers. The two dimensional Laplacian is approximated by

$$(\Delta u)_{i,j} = \frac{u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{i,j}}{h^2}. \tag{4.543}$$

The eigenvalue problem thus becomes a matrix problem $Lu = \lambda u$ where u is a vector of variables, and the entries of L can be read off from Eq. (4.543). For this the matrix $u_{i,j}$ of variables has to be reshaped to a vector. The finite difference method is easy to program from scratch, but almost never the best choice.

In contrast, the finite element method is almost always the most efficient, but very difficult to program. One has to rely on professional programs, such as the FEM toolbox of MATLAB. The region Ω is structured by a triangulation. Figure 4.29 is an example. Each node is associated with the field value there, a variable. Again,

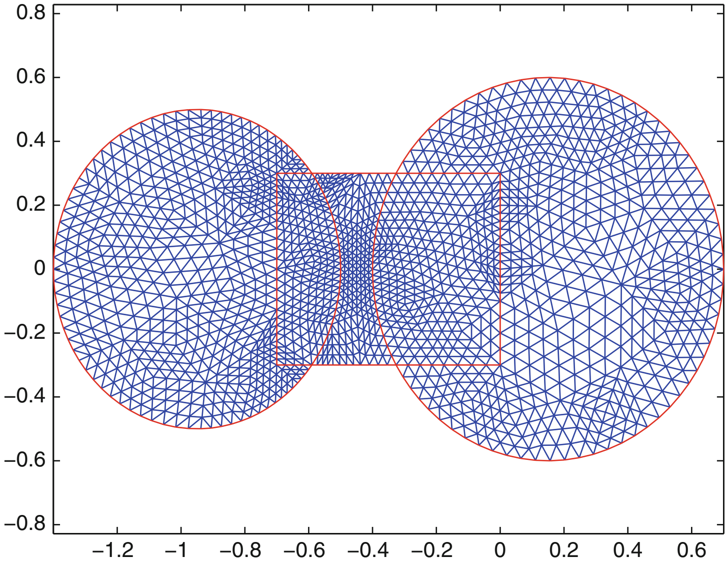

Fig. 4.29 A very crude approximation to the back of a violin. Its eigenmodes are calculated by the finite element method. This is the mesh of *triangles* by which the region Ω is approximated

the eigenvalue problem is reduced to a matrix problem $Lu = \lambda u$. However, one is not bound to equal spacing. The triangulation may be refined where necessary, even automatically.

We have calculated, by the finite element method FEM, the second lowest eigenmode of a membrane which resembles the back of a violin. The approximation is really very crude. First of all, the violin's resonance body is more than the back. Second, the back is not flat as was assumed here. Third, the back is made of wood which behaves very an-isotropically. Its wave equation is certainly not so simple as Eq. (4.526). Fourth, the back is not just wood, but varnished. It is well-known that the famous families Amati, Stradivari and Guarnieri of Cremona in Italy zealously kept the secret of their varnishes. See Fig. 4.30.

Again, we must stop here although there is much more to say about vibrating membranes and plates.

Let us finally turn to a mathematical problem. The wave equation (4.526) refers to a region Ω. Different regions will result in different sets of eigenvalues ω_n, or spectra. Apart from symmetry operations like mirroring, the spectra of different Ω shapes are different. Are they? This question has been condensed into the question *Can one hear the shape of a drum*?, an old standing problem. It was answered by Mark Kac [4] to the negative. There are differing regions Ω which give rise to the same spectrum.

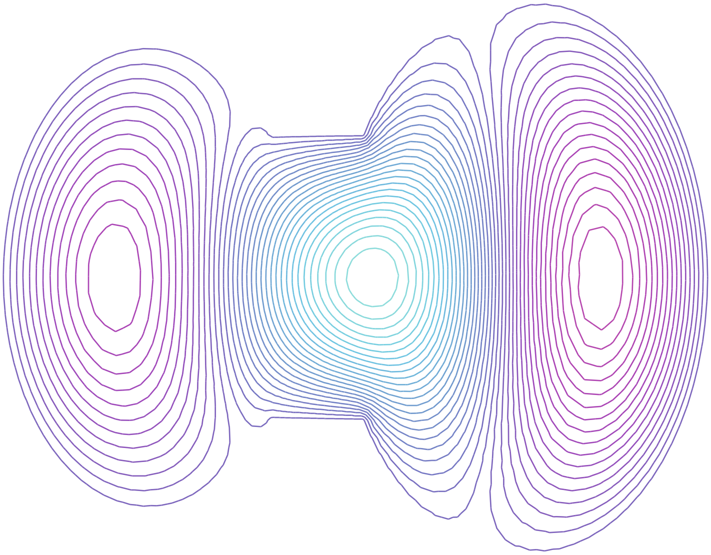

Fig. 4.30 The second excited mode of a crude model for a violin back as calculated with the finite element method. See Fig. 4.29 for the decomposition of Ω into finite elements

4.28 White Dwarfs

A normal star collapses if it has burnt most of its hydrogen into helium. In its core, nuclear reactions are then ignited which fuse helium into carbon and oxygen.[61] Thereby the star blows up and becomes a red giant, such as Betelgeuse. When the core is small enough, no further fusion reactions are possible and the core blows off its hull. The dense core is a plasma of carbon and oxygen nuclei and electrons. It is the degeneracy pressure of the electron gas which stabilizes the core, a white dwarf. It is called a dwarf because its diameter is comparable to that of the earth, although its mass is comparable to that of the sun. It is a white dwarf because the remaining internal energy is radiated off by a small surface with a high color temperature. White dwarfs cool down more and more until they become invisible. In our vicinity, eight out of hundred stars are still visible white dwarfs, and many more are no more visible.

The best known is the companion of Sirius. Before being spotted optically, it was predicted to be responsible for the Kepler orbit of Sirius, or Sirius A. This star has 2.1 sun masses and is 25 times as bright as the sun. Sirius B, the white dwarf companion, has a mass comparable to that of the sun, but it is 400 times fainter.

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[61] These two nuclei have rather large binding energies per nucleon, they are made up of three resp. four helium nuclei. Iron has the largest binding energy, it is the most common remnant of supernovae.

4.28.1 The Model

Since this is not a textbook on astrophysics, we restrict ourselves to the essentials. We assume that the model white dwarf is electrically neutral everywhere, that it does not rotate, and that it is close to its final stage which is described by zero temperature. Gravitation is balanced by the degeneracy pressure of electrons only which we assume to be free particles. We assume rotational symmetry such that fields depend on r only, the distance from the star's center. We treat the electrons non-relativistically.

Denote by

$$M(r) = 4\pi \int_0^r \mathrm{d}s\, s^2 \varrho(s) \tag{4.544}$$

the mass within a sphere of radius r. $\varrho = \varrho(r)$ denotes mass density, as usual. The gravitational force per unit volume at distance r is given by

$$f(r) = -G\, \frac{\varrho(r) M(r)}{r^2}, \tag{4.545}$$

where G denotes the universal gravitational constant.[62] The star is gravitationally stable if the negative pressure gradient $p'(r)$ and $f(r)$ add up to zero everywhere:

$$p'(r) = f(r). \tag{4.546}$$

This is the momentum balance equation for a resting fluid medium within its own gravitational field.

4.28.2 Equation of State

To proceed, we must relate pressure with mass density. Denote by n the density of electrons and by μ their chemical potential. They are related by

$$n(T,\mu) = \int_0^\infty \mathrm{d}\epsilon\, z(\epsilon)\, \frac{1}{\mathrm{e}^{(\epsilon-\mu)/k_\mathrm{B}T} + 1}, \tag{4.547}$$

because electrons are fermions.

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[62] The gravitational force of a rotationally symmetric mass distribution is the same as that of a point mass at the origin. Only mass which is closer to the origin contributes. This finding goes back to Newton.

$z = z(\epsilon)$ is the number of states per unit energy and per unit volume, of a single particle. For free particles,

$$z(\epsilon) = \frac{1}{\pi^2} \left\{ \frac{2m}{\hbar^2} \right\}^{3/2} \sqrt{\epsilon} \tag{4.548}$$

describes the density of states. We have set $\epsilon = (\hbar k)^2/2m$ and used the well-known result that the phase space volume $\mathrm{d}^3k\,\mathrm{d}^3x/(2\pi\hbar)^3$ corresponds to one state. The pressure of such a gas of non-interacting fermions is

$$p(T,\mu) = \frac{2}{3} \int_0^\infty \mathrm{d}\epsilon\, z(\epsilon)\, \frac{\epsilon}{\mathrm{e}^{(\epsilon-\mu)/k_\mathrm{B}T} + 1}. \tag{4.549}$$

The limit $T \to 0$ results in

$$n(0,\mu) = \int_0^\mu \mathrm{d}\epsilon\, z(\epsilon) = \frac{2}{3\pi^2} \left\{ \frac{2m}{\hbar^2} \right\}^{3/2} \mu^{3/2} \tag{4.550}$$

and

$$p(0,\mu) = \frac{2}{3} \int_0^\mu \mathrm{d}\epsilon\, z(\epsilon)\, \epsilon = \frac{4}{15\pi^2} \left\{ \frac{2m}{\hbar^2} \right\}^{3/2} \mu^{5/2}. \tag{4.551}$$

By eliminating the chemical potential μ we arrive at the following relation between pressure and particle density:

$$p = a\, \frac{\hbar^2}{m}\, n^{5/3}. \tag{4.552}$$

Indeed, this is an energy density, or a pressure. The numerical factor has the value

$$a = \frac{1}{5} \left(\frac{3\pi^2}{2} \right)^{2/3} = 1.2058. \tag{4.553}$$

Now, carbon and oxygen contain equally many protons as neutrons. Hence one electron is related with approximately $2m_\mathrm{p}$, twice the mass of a proton. Since we assume that matter is locally neutral, the searched for relation between pressure and mass density is given by

$$p = a\, \frac{\hbar^2}{m_\mathrm{e}} \left\{ \frac{\varrho}{2m_\mathrm{p}} \right\}^{5/3}. \tag{4.554}$$

Besides a numerical constant a the mass m_e and m_p of electrons and protons respectively show up as well as Planck's constant $\hbar$. This material equation is of truly quantum-mechanical origin.

4.28.3 Orders of Magnitude

Let us consider a white dwarf consisting of $N = 10^{57}$ nucleons, roughly 0.85 sun masses. Its radius is denoted by R. A very rough estimate is

$$p' \approx \frac{\hbar^2}{m_\mathrm{e}} \frac{N^{5/3}}{R^5} \frac{1}{R} \tag{4.555}$$

for the pressure gradient and

$$f \approx G \frac{m_\mathrm{p}^2 N^2}{R^2} \frac{1}{R^3} \tag{4.556}$$

for the gravitational force per unit volume. Equating these estimates yields

$$R \approx \frac{\hbar^2}{m_\mathrm{e} m_\mathrm{p}^2 G} N^{-1/3}, \tag{4.557}$$

which amounts to 6,500 km. Note that this value—about the radius of our earth—is determined by the universal gravitational constant G, the masses of electrons and protons, Planck's constant $\hbar$, and the number N of nucleons which make up a normal star like the sun. Note also that less massive white dwarfs are larger.

4.28.4 Numerical Solution

Let us measure length in units of $\ell_* = R$, mass in units of $M_* = m_\mathrm{p} N$. We likewise introduce $\varrho_* = M_*/R^3$ and $p_* = \hbar^2 N^{5/3}/m_\mathrm{e} R^4$ as units of mass density and pressure, respectively. In these units[63] the equations under study read

$$p' = -\frac{M\varrho}{r^2}, \tag{4.558}$$

$$M' = 4\pi r^2 \varrho, \tag{4.559}$$

and

$$p = b\varrho^{5/3}. \tag{4.560}$$

$b = 0.3798$ is an abbreviation for $2^{-5/3}a$ where a was defined in Eq. (4.553). Note that (4.558) and (4.559) are dimension-less equations suitable for numerical treatment.

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[63] The distance from the star's center is rR_*, and so on. All physical quantities are now dimensionless.

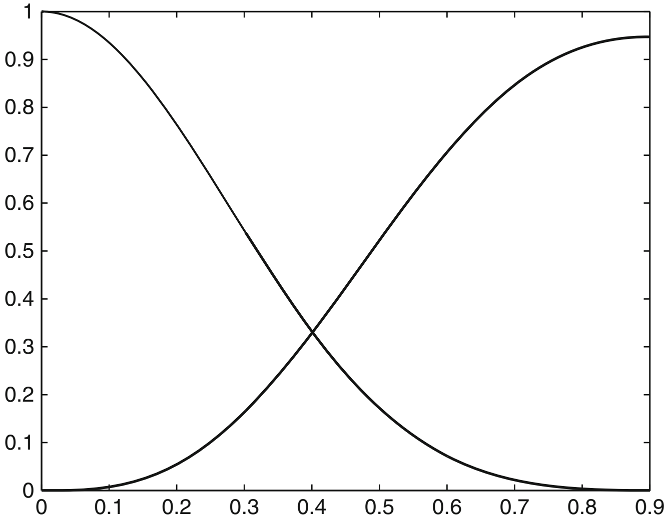

Fig. 4.31 Pressure p (decreasing) and mass M (increasing) of a white dwarf vs. distance r from the *center* in natural units. We have assumed zero temperature, two nucleons per electron which are treated non-relativistically. $r = 1$ corresponds to 6,500 km, $M = 1$ to 0.85 sun masses

We have integrated this coupled system of two ordinary differential equations with the initial conditions $p(0) = 1.0$ and $M(0) = 0$. Figure 4.31 depicts the result.

4.28.5 Remarks

Historically, the fate of stars was a subject of much discussion and speculation. What would happen if they cool down so that thermal pressure could no longer stabilize them from gravitational collapse? It was a very short time span when many old riddles were solved. In 1926 Erwin Schrödinger was able to calculate the stationary states of the hydrogen atom. Before, in classical electrodynamics, moving charges would radiate off energy, an electrostatic counterpart of the Kepler system of two attracting masses was not possible.

Also in 1926, Enrico Fermi published a paper on the quantum-statistical behavior of identical particles with half-integer spin (now called fermions). In particular, the Pauli exclusion principle proved to be a limiting case for $T = 0$, the periodic system of elements could be explained as well as the basic properties of solids (isolators, conductors).

In the same year 1926 R.H. Fowler recognized the relevance of quantum mechanics for astrophysics. Besides thermal pressure (ideal gas law), there is a degeneracy pressure which derives from the fact that fermions, such as electrons, dislike to be at the same location. In a paper "On dense matter" he wrote that a white dwarf is nothing else but a giant molecule. Only a short time later S. Chandrasekhar calculated the limiting mass of a white dwarf by taking the relativist energy-momentum relation into account (which won him a Nobel prize).

This Chandrasekhar limit[64] has turned out to be of utmost importance in the field of experimental cosmology. There are binary star systems where one member is a white dwarf. The other member is surrounded by a large cloud of matter which feeds the white dwarf. The white dwarf continuously sucks in matter until it reaches the Chandrasekhar limit. Then it suffers a supernova explosion with a characteristic luminosity versus time pattern. All such type Ia supernovae are alike, they serve as a standard candle. The *absolute* luminosity is always the same, but the *apparent* luminosity depends on distance r by a $1/r^2$ law. Therefore, type Ia supernova allow to determine cosmic distance.

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[64] The mass of a white dwarf cannot exceed 1.44 sun masses.

Appendix A
Fields

A physical quantity which depends on time and space is described by a field. The quantity itself may be a scalar, a vector, or a second-rank tensor. Practically everything in this book is a field.

Fields, although they describe physical properties, must be represented by mathematical functions which depend on a time coordinate t and three space coordinates $\boldsymbol{x} = (x_1, x_2, x_3)$ with respect to an inertial system. Since there are many inertial systems, the same physical field will be represented by many mathematical fields.

In the section on *Covariance* we discuss how to make sure that different inertial systems and therefore different field representations describe the same physical situation. Relativistic effects are not touched upon in this book, therefore the non-relativistic limit is quite sufficient.

Section *Differentiating Fields* covers those differentiation operations which guarantee that covariant fields are mapped into covariant fields: gradient, divergence, and curl.

In section *Paths, Surfaces and Volumes* we discuss how to describe one, two and tree dimensional manifolds of three dimensional space. These are paths, surfaces and volumes, respectively.

We show in *Integrating Fields* how to define path, surface and volume integrals of scalar and vector fields and examine generalizations of the fundamental theorem of calculus.

The local center of mass velocity field $\boldsymbol{v}$ plays a particular role in Continuum Physics. Some useful notions and formulas referring to the velocity field are presented in section *More on Fields*. Some of the arguments presented here were already put forward in section *Convection and Conduction* of Chap. 1.

Fields are functions $f = f(t, x_1, x_2, x_3)$. Partial differentiation with respect to the first argument is denoted by ∂_t in operator notation. Likewise, differentiation with respect to x_1, x_2, x_3 is denoted by $\partial_1, \partial_2, \partial_3$. We adhere to Einstein's convention: if, within a term, an index $i = 1, 2, 3$ occurs twice, a sum over it is silently understood, such as $a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$.

P. Hertel, *Continuum Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-642-29500-3,

A.1 Covariance

Theoretical physics tries to build bridges between the world of things and events on the one and mathematics on the other hand. We have to translate from the real world to mathematics, do our calculations according to the laws of mathematics, and re-translate the results to the real world. A physicist has been educated within this scheme of thinking that he hardly notices it any more.

Just think about the length of an object. You must specify a number and a reference length, meters say. "He measures 1.85" may be correct within a certain context, but "he measures 1.85 m" is better, or "he measures 185 cm". This example should have made clear that the translation of physical properties to numbers requires a reference system, and also, that there are many of them, such as meter, centimeter, inches, typographical points, and so forth.

A.1.1 Inertial Systems of Reference

Fields describe events, physical properties which are answers to what? when? and where? questions. Time is measured by a good clock which, if events occur periodically, always indicates the same period. Locations are characterized by referring to a coordinate system. We here restrict ourselves to Cartesian coordinates, three identical measuring rods at right angles. The marks on such a rod are equally spaced which can be verified by translating one with respect to another. If two points A and B are characterized by coordinates (a_1, a_2, a_3) and (b_1, b_2, b_3), their distance is

$$d = \sqrt{(b_1 - a_1)^2 + (b_2 - a_2)^2 + (b_3 - a_3)^2}, \tag{A.1}$$

the Pythagoras formula in three-dimensional space. Equation (A.1) holds true only for a Cartesian coordinate system.

Since Galileo Galilei we know that there are preferred systems, so called inertial systems. Normally, bodies are inert in the sense of "lazy", they do not change their state of motion unless forced to do so. A body which is not acted upon by a force travels on a trajectory

$$\boldsymbol{x}(t) = \boldsymbol{x}_0 + t\,\boldsymbol{v}. \tag{A.2}$$

Equation (A.2) characterizes an inertial system Σ of reference. A rotating coordinate system or a more and more retarding clock will not give rise to linear trajectories like Eq. (A.2).

There are inertial systems of reference, however, there are many of them. If the when? and where? questions of a typical event are answered by t, x_1, x_2, x_3 with respect to Σ and by t', x_1', x_2', x_3' with respect to Σ', the following relation must hold true:

$$t = t' + \tau \text{ and } \boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'. \tag{A.3}$$

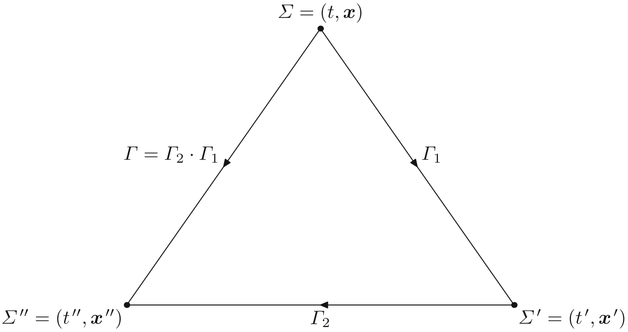

Fig. A.1 Sending the inertial system Σ into Σ' by Γ_1 and then, by Γ_2, to Σ''. This is the same as sending Σ to Σ'' by Γ

Here R is an orthogonal matrix,

$$RR^\dagger = R^\dagger R = I \text{ or } R_{ij} R_{kj} = \delta_{ik}. \tag{A.4}$$

An orthogonal matrix guarantees that the distance between two points is the same if calculated with primed or unprimed coordinates.

Inserting a trajectory Eq. (A.2) into Eq. (A.3) results in another trajectory where time and location are related by linear functions.

Equation (A.3) describes a Galilei transformation $\Gamma = \{\tau, \boldsymbol{a}, R, \boldsymbol{u}\}$.

If Γ_1 sends $(t, \boldsymbol{x})$ to $(t', \boldsymbol{x}')$ and Γ_2 sends $(t', \boldsymbol{x}')$ to $(t'', \boldsymbol{x}'')$, the transformation $\Gamma = \Gamma_2 \cdot \Gamma_1$ directly sends $(t, \boldsymbol{x})$ to $(t'', \boldsymbol{x}'')$. We easily work out

$$\Gamma = \Gamma_2 \cdot \Gamma_1 = \{\tau_2 + \tau_1, \boldsymbol{a}_2 + R_2\boldsymbol{a}_1, R_2 R_1, \boldsymbol{u}_2 + R_2\boldsymbol{u}_1\}. \tag{A.5}$$

This is indeed a Galilei transformation because the product $R_2 R_1$ of two orthogonal matrices is again an orthogonal matrix. See Fig. A.1 for a sketch.

Galilei transformations form a group. There are various subgroups:

- Time translations: $\Gamma = \{\tau, 0, I, 0\}$
- Spatial translations: $\Gamma = \{0, \boldsymbol{a}, I, 0\}$
- Rotations: $\Gamma = \{0, 0, R, 0\}$
- Proper rotations: $\Gamma = \{0, 0, R, 0\}$ where $\det(R) = 1$
- Proper Galilei transformations: $\Gamma = \{0, 0, I, \boldsymbol{u}\}$

Because of $\{0, \mathbf{0}, I, \boldsymbol{u}_2\} \cdot \{0, \mathbf{0}, I, \boldsymbol{u}_1\} = \{0, \mathbf{0}, I, \boldsymbol{u}_2 + \boldsymbol{u}_1\}$ we conclude that velocities add as vectors. This is in disagreement with the fact that the velocity c of light is always the same. Galilei transformations are approximations for small relative velocities. A fully relativistic description of continuum mechanics is not within the scope of this book, it is not required.

A.1.2 Tensor Fields

One and the same event is characterizes by coordinates $(t, \boldsymbol{x})$ with respect to an inertial system Σ and by $(t', \boldsymbol{x}')$ when referring to another inertial system Σ'. If the event is associated with a property which can be expressed by a single number $S = S(t, \boldsymbol{x})$, we speak of a scalar field. This is a function of four arguments. With respect to the inertial system Σ' the same physical field is expressed by a different function, namely $S' = S'(t', \boldsymbol{x}')$. Both functions shall represent the same physical field, therefore

$$S(t, \boldsymbol{x}) = S'(t', \boldsymbol{x}')) \tag{A.6}$$

must hold true, where $\Gamma = \{\tau, \boldsymbol{a}, R, \boldsymbol{u}\}$ transforms from Σ' to Σ according to Eq. (A.3).

We speak of a vector field if the event is associated with a vector $\boldsymbol{V}$. A vector field is represented by three functions $V_i = V_i(t, \boldsymbol{x})$ with respect to the inertial coordinate system Σ and by three different functions V_i' with respect to Σ' such that

$$V_i(t, \boldsymbol{x}) = R_{ij} V_j'(t', \boldsymbol{x}') \tag{A.7}$$

holds true.

A tensor field T_{ij} in the narrow sense of the word has two indexes and transforms as

$$T_{ij}(t, \boldsymbol{x}) = R_{ik} R_{jl} T_{kl}'(t', \boldsymbol{x}'). \tag{A.8}$$

A tensor field in the wider sense has $n = 0, 1, 2 \dots$ indexes and transforms as above, with one R matrix for each index. The number of indexes is the rank of the tensor. Hence, a scalar field is a rank zero tensor field, a vector field is a tensor field of rank 1, a proper tensor field has two indexes, and so forth.

Physical laws must be formulated as equations $T(t, \boldsymbol{x}) = 0$ where T stands for a tensor field of a certain rank. Then, and only then, the expression is true for all inertial systems and expresses the same physical information.

Here are some recipes how to construct valid tensor expressions:

- A linear combination of two tensors of the same kind is again such a tensor, such as $C_{ij} = \alpha A_{ij} + \beta B_{ij}$
- The product of a scalar and a tensor field is again such a tensor field, such as $C_{ij}(t, \boldsymbol{x}) = S(t, \boldsymbol{x}) T_{ij}(t, \boldsymbol{x})$
- The product $C_{ij} = A_i B_j$ of two vector fields $\boldsymbol{A}$ and $\boldsymbol{B}$ is a tensor field
- Summing over a pair of identical indexes results in a tensor of rank minus two, such as in $S = A_i B_i$ where $\boldsymbol{A}$ and $\boldsymbol{B}$ are vector fields and S is a scalar field
- The Kronecker symbol δ_{ij} is a constant tensor field of rank 2, because of $R_{ik} R_{jl} \delta_{kl} = \delta_{ij}$

- The Levi-Civita symbol ϵ_{ijk} is a constant pseudo-tensor of rank three. Because of[1]
$$R_{il}\,R_{jm}R_{kn}\epsilon_{lmn} = \det(R)\,\epsilon_{ijk} \tag{A.9}$$
it transforms as a rank three tensor if $\det(R) = 1$, that is for proper rotations. It acquires a minus sign for improper rotations. Such objects are called pseudo-scalars, pseudo-vectors, and so forth
- If $\boldsymbol{A}$ and $\boldsymbol{B}$ are proper vectors, then $\boldsymbol{C} = \boldsymbol{A} \times \boldsymbol{B}$ transforms as a pseudo-vector, because of $C_i = \epsilon_{ijk} A_j B_k$. However, if $\boldsymbol{A}$ is a proper vector and $\boldsymbol{B}$ a pseudo-vector, then $\boldsymbol{C}$ will transform as a proper vector

A.2 Differentiating Fields

We show that the time derivative ∂_t does *not* behave as a scalar. We shall postpone this problem to section *More on Fields* of this appendix where we justify the decomposition of current densities into a convection and a conduction contribution. The three partial differentiation operators ∂_i with respect to location transform as a proper vector giving rise to gradient, divergence, and curl fields.

A.2.1 Time Derivative

Consider a scalar field. When changing from one inertial system to another by a Galilei transformation $\Gamma = \{\tau, \boldsymbol{a}, R, \boldsymbol{u}\}$ according to Eq. (A.3), the field transforms as described by Eq. (A.6), that is

$$S'(t',\boldsymbol{x}') = S(t,\boldsymbol{x}) = S(\tau + t', \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'). \tag{A.10}$$

The partial derivative with respect to t', i.e., by keeping $\boldsymbol{x}'$ fixed, results in

$$\partial_{t'} S'(t',\boldsymbol{x}') = \partial_t S(t,\boldsymbol{x}) + u_i \partial_i S(t,\boldsymbol{x}). \tag{A.11}$$

We conclude that the partial time derivative of a scalar field does *not* transform as a scalar under Galilei transformations. Put otherwise, ∂_t is not a scalar.

---

[1] Equation (A.9) holds true for any 3 × 3 matrix R. In fact, it defines its determinant.

A.2.2 *Gradient*

Consider a scalar field S which is characterized by Eq. (A.10). We differentiate it with respect to x'_i treating t' as constant. The result is

$$\frac{\partial S'}{\partial x'_i} = \frac{\partial S(\tau + t', \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t')}{\partial x_j} R_{ji}, \tag{A.12}$$

which we abbreviate to

$$\partial'_i S'(t', \boldsymbol{x}') = R_{ji} \partial_j S(t, \boldsymbol{x}) = (R^\dagger)_{ij} \partial_j S(t, \boldsymbol{x}). \tag{A.13}$$

Because of $RR^\dagger = I$ this may be rewritten as

$$\partial_i S(t, \boldsymbol{x}) = R_{ij} \partial'_j S'(t', \boldsymbol{x}'). \tag{A.14}$$

$G_i = \partial_i S$ is the gradient of a scalar field S, it transforms as a proper vector field.

A.2.3 *Divergence*

The above finding says that the differentiation operator ∂_i transforms as a vector. So, if V_i is a vector field, then $\partial_j V_i$ transforms as a tensor, and the same applies to tensors of higher rank. By what has been said before, the divergence $D = \partial_i V_i$ of a vector field will transform as a scalar field:

$$\partial_i V_i(t, \boldsymbol{x}) = \partial'_i V_i{}'(t', \boldsymbol{x}'). \tag{A.15}$$

The divergence of the gradient of a scalar field S, namely

$$\Delta S = \partial_i \partial_i S, \tag{A.16}$$

is a scalar field as well. Δ denotes the Laplacian operator.

A.2.4 *Curl*

If V_i is a vector field, its curl is defined as

$$C_i = \epsilon_{ijk} \partial_j V_k. \tag{A.17}$$

It transforms as a pseudo vector field:

$$C_i(t,\boldsymbol{x}) = \det(R)\; R_{ij}\, C'_j(t',\boldsymbol{x}') \tag{A.18}$$

in familiar notation.

A curl field is always divergence free, because of

$$\partial_i C_i = \epsilon_{ijk} \partial_i \partial_j V_k = 0. \tag{A.19}$$

While $\partial_i \partial_j$ is symmetric, the Levi-Civita symbol ϵ_{ijk} is antisymmetric when interchanging i and j. Summing over i and j results in zero.

For the same reason, the curl of a gradient $G_i = \partial_i S$ always vanishes,

$$\epsilon_{ijk} \partial_j G_k = \epsilon_{ijk} \partial_j \partial_k S = 0. \tag{A.20}$$

A.3 Paths, Surfaces and Volumes

Fields, living in a three dimensional space and depending on time, can be integrated over one-, two-, or three-dimensional manifolds, namely paths, surfaces and volumes. We explain how these manifolds are defined. The time argument t is kept constant in this and following sections, so we drop it entirely.

A.3.1 Paths

A path $\mathcal{C}$ is parameterized by a differentiable mapping of an interval into three dimensional space,

$$u \to \boldsymbol{\xi}(u) \text{ where } u \in [u_0, u_1] \text{ and } u_0 < u_1. \tag{A.21}$$

$\boldsymbol{x}_0 = \boldsymbol{\xi}(u_0)$ is the start point, $\boldsymbol{x}_1 = \boldsymbol{\xi}(u_1)$ the end point.

Now, assume a monotonously increasing function f which maps the interval $[\bar{u}_0, \bar{u}_1]$ onto $[u_0, u_1]$. We define by

$$\bar{\boldsymbol{\xi}}(\bar{u}) = \boldsymbol{\xi}(u) = \boldsymbol{\xi}(f(\bar{u})) \tag{A.22}$$

the composition $\bar{\boldsymbol{\xi}} = \boldsymbol{\xi} \circ f$. If $\bar{u}$ runs from $\bar{u}_0$ to $\bar{u}_1$, $\bar{\boldsymbol{\xi}}(\bar{u})$ runs from $\boldsymbol{x}_0$ to $\boldsymbol{x}_1$ on the same path as above, and in the same order. We say that $u \to \boldsymbol{\xi}(u)$ and $\bar{u} \to \bar{\boldsymbol{\xi}}(\bar{u})$ are equivalent parameterizations.

We see that the same path can be parameterized by different functions $\boldsymbol{\xi}(u)$, $\bar{\boldsymbol{\xi}}(\bar{u})$, and so forth. In fact, the class of all equivalent parameterizations *is* the path. See Fig. A.2 for a sketch.

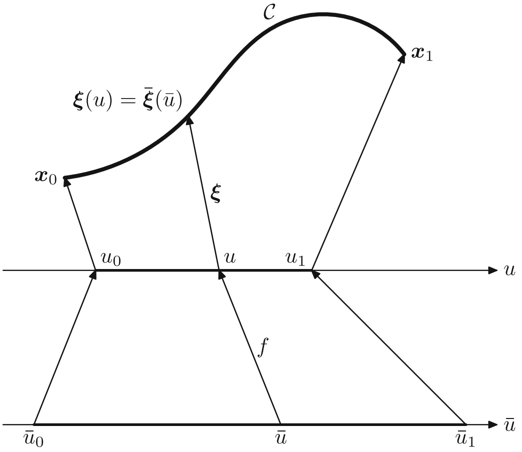

Fig. A.2 Two different parameterizations of the same path $\mathcal{C}$

So far we demanded that the parameterization be differentiable. This can be relaxed. Consider two paths $\mathcal{C}'$ and $\mathcal{C}''$. The former starts at $\boldsymbol{x}'_0$ and ends at $\boldsymbol{x}'_1$, the latter at $\boldsymbol{x}''_0$ and $\boldsymbol{x}''_1$. If it happens that the end point of $\mathcal{C}'$ coincides with the start point of $\mathcal{C}''$, we may join them to one path $\mathcal{C} = \mathcal{C}' + \mathcal{C}''$. $\mathcal{C}$ is obviously continuous and consist of two differentiable pieces. It starts at $\boldsymbol{x}'_0$ and ends at $\boldsymbol{x}''_1$. In general, a path is made up of finitely many differentiable pieces.

If the start and end points of a path are the same, we speak of a closed path.

The boundary of a path $\mathcal{C}$ which begins at $\boldsymbol{x}_\mathrm{s}$ and ends at $\boldsymbol{x}_\mathrm{e}$ is denoted by $\partial\mathcal{C}$. It is the ordered set $\{\boldsymbol{x}_\mathrm{s}, \boldsymbol{x}_\mathrm{e}\}$.

For each differential piece we can define the tangent vector by

$$\boldsymbol{t}(u) = \frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}u}. \tag{A.23}$$

If we calculate the tangent vector with respect to another parameterization we find

$$\bar{\boldsymbol{t}}(\bar{u}) = \frac{\mathrm{d}u(\bar{u})}{\mathrm{d}\bar{u}}\,\boldsymbol{t}(u). \tag{A.24}$$

Hence, $\bar{\boldsymbol{t}}$ and $\boldsymbol{t}$ are parallel,[2] although not equal. This means that the tangential unit vector does not depend on the particular parameterization, it is a property of the path.

There is a particular parameterization $s \to \boldsymbol{\xi}(s)$ such that $|\boldsymbol{t}(s)| = 1$ holds everywhere. In this case we call s the arc length. If the starting point of a path $\mathcal{C}$ is characterized by s_0 and the end point by s_1, the path length of $\mathcal{C}$ is $\ell = s_1 - s_0$.

---

[2] Note that $\mathrm{d}u/\mathrm{d}\bar{u}$ is positive.

A circle in the x, y-plane may serve as an example:

$$s \to \boldsymbol{\xi}(s) = R \begin{pmatrix} \cos(s/R) \\ \sin(s/R) \\ 0 \end{pmatrix} \text{ for } s \in [0, 2\pi R]. \tag{A.25}$$

Its tangent vector is given by

$$\boldsymbol{t}(s) = \begin{pmatrix} -\sin(s/R) \\ \cos(s/R) \\ 0 \end{pmatrix}, \tag{A.26}$$

a unit vector. Hence s serves as the arc length. The circumference (path length) of the circle is $2\pi R$. Note that the circle is a closed path.

Assume we use the arc length s as a parameter. We may write

$$\frac{\mathrm{d}^2\boldsymbol{\xi}(s)}{\mathrm{d}s} = \frac{\mathrm{d}\boldsymbol{t}(s)}{\mathrm{d}s} = \kappa(s)\boldsymbol{n}(s). \tag{A.27}$$

The normal vector $\boldsymbol{n}$ should have unit length which defines the curvature $\kappa(s) \geq 0$. The radius of curvature at s is given by $R(s) = 1/\kappa(s)$, it is likewise zero or positive (possibly infinite). Because of

$$0 = \frac{\mathrm{d}}{\mathrm{d}s}1 = \frac{\mathrm{d}}{\mathrm{d}s}\boldsymbol{t}(s) \cdot \boldsymbol{t}(s) = 2\boldsymbol{t}(s) \cdot \frac{\mathrm{d}\boldsymbol{t}(s)}{\mathrm{d}s} \tag{A.28}$$

the normal vector $\boldsymbol{n}$ is perpendicular to the tangent vector $\boldsymbol{t}$. The normal vector points towards the origin of a circle of radius R which locally approximates the curve in second order.

The normal vector $\boldsymbol{n}(s)$ for the circle Eq. (A.25) turns out to

$$\frac{\mathrm{d}}{\mathrm{d}s}\begin{pmatrix} -\sin(s/R) \\ \cos(s/R) \\ 0 \end{pmatrix} = \frac{1}{R}\boldsymbol{n}(s) \text{ where } \boldsymbol{n} = \begin{pmatrix} -\cos(s/R) \\ -\sin(s/R) \\ 0 \end{pmatrix}. \tag{A.29}$$

For a circle of radius R the radius of curvature $R(s)$ is the same everywhere, namely R.

A.3.2 Surfaces

We repeat the above pattern for a two-dimensional manifold. The rectangle $\mathcal{R} = [u_0, u_1] \times [v_0, v_1]$ is mapped by three differentiable functions $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v)$ into the three-dimensional space. Such a two-dimensional manifold is called a surface $\mathcal{A}$.

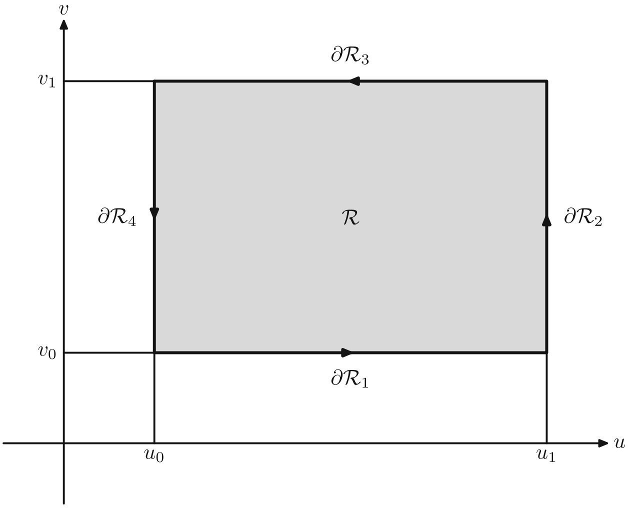

Fig. A.3 Rectangle $\mathcal{R} = [u_0, u_1] \times [v_0, v_1]$ and the four pieces of its boundary $\partial\mathcal{R}$

The boundary of $\mathcal{R}$ consists of four pieces, $\partial\mathcal{R} = \partial\mathcal{R}_1 + \partial\mathcal{R} + \partial\mathcal{R}_3 + \partial\mathcal{R}_4$. It is a path which runs counter-clockwise, see Fig. A.3.

Again, we may choose another rectangle $\bar{\mathcal{R}} = [\bar{u}_0, \bar{u}_1] \times [\bar{v}_0, \bar{v}_1]$. Let $u_1 = f_1(\bar{u}, \bar{v})$ and $u_2 = f_2(u, v)$ be two differentiable functions which map $\bar{\mathcal{R}}$ onto $\mathcal{R}$. We require the mapping to be invertible. This is the case if the so-called Jacobian

$$\frac{\partial(f_1, f_2)}{\partial(\bar{u}, \bar{v})} = \det \begin{pmatrix} \dfrac{\partial f_1}{\partial u} & \dfrac{\partial f_2}{\partial u} \\ \dfrac{\partial f_1}{\partial v} & \dfrac{\partial f_2}{\partial v} \end{pmatrix} \tag{A.30}$$

vanishes nowhere. We also restrict the mapping by demanding that the orientation of the boundary $\partial\bar{\mathcal{R}}$ is counter-clockwise.

The boundary $\partial\mathcal{A}$ of a surface $\mathcal{A}$ is the mapping by $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v)$ of the boundary $\partial\mathcal{R}$. It inherits its orientation, and this is also true for another parameterization $\bar{\boldsymbol{\xi}} = \bar{\boldsymbol{\xi}}(\bar{u}, \bar{v})$.

We now have two tangential vectors, namely

$$\boldsymbol{t}_1(u, v) = \frac{\partial \boldsymbol{\xi}(u, v)}{\partial u} \text{ and } \boldsymbol{t}_2(u, v) = \frac{\partial \boldsymbol{\xi}(u, v)}{\partial v}. \tag{A.31}$$

They are nowhere parallel. They span the tangential plane which consists of all linear combinations of $\boldsymbol{t}_1(u, v)$ and $\boldsymbol{t}_2(u, v)$.

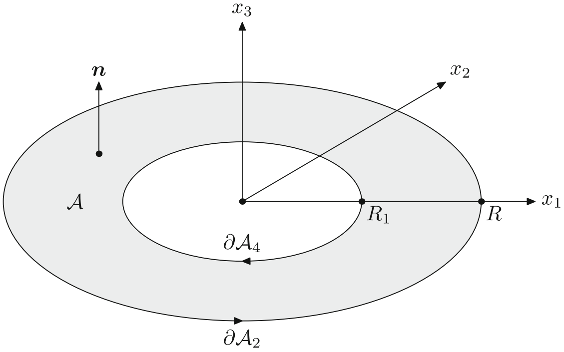

Fig. A.4 $\mathcal{A}$ is a larger spherical disk without a smaller one (*gray*). The boundary consists of two disjoint closed paths $\partial\mathcal{A}_2$ and $\partial\mathcal{A}_4$. The normal vector $\boldsymbol{n}$ is the same everywhere

Because of

$$\bar{\boldsymbol{t}}_1 = \frac{\partial u}{\partial \bar{u}}\boldsymbol{t}_1 + \frac{\partial v}{\partial \bar{u}}\boldsymbol{t}_2 \text{ and } \bar{\boldsymbol{t}}_2 = \frac{\partial u}{\partial \bar{v}}\boldsymbol{t}_1 + \frac{\partial v}{\partial \bar{v}}\boldsymbol{t}_2 \tag{A.32}$$

we see that this plane is the same for all parameterizations. Therefore, the normal vector[3]

$$\boldsymbol{n}(u,v) = \frac{\boldsymbol{t}_1(u,v)\times\boldsymbol{t}_2(u,v)}{|\boldsymbol{t}_1(u,v)\times\boldsymbol{t}_2(u,v)|} \tag{A.33}$$

is well defined, irrespective of the parameterization.

In general, a surface consists of finitely many differentiable pieces which are sewn together in such a way that it is continuous.

A surface is closed if it has no boundary.

Let us illustrate all this by an example:

$$\boldsymbol{\xi}(r,\phi) = \begin{pmatrix} r\cos\phi \\ r\sin\phi \\ 0 \end{pmatrix} \text{ for } r \in [R_1, R] \text{ and } \phi \in [0, 2\pi]. \tag{A.34}$$

The boundary consists of four pieces (see Fig. A.3).

- $\partial\mathcal{A}_1$: A straight line from $(R_1, 0)$ to $(R, 0)$ in the x, y plane.
- $\partial\mathcal{A}_2$: A counter-clockwise circle with radius R around the coordinate center.
- $\partial\mathcal{A}_3$: A straight line from $(R, 0)$ to $(R_1, 0)$.
- $\partial\mathcal{A}_4$: A clockwise circle with radius R_1 around the coordinate center.

The first and the third contribution drop out, their sum is the null path. See Fig. A.4 for a sketch.

Note that, with $R_1 \to 0$, the inner circle becomes the null path, and the surface is a plane disk of radius R.

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[3] Not to be confused with the normal vector of a path.

A.3.3 Volumes

A volume $\mathcal{V}$, a three-dimensional manifold, is described by a differentiable mapping $\boldsymbol{\xi}$ of a cuboid $\mathcal{Q}$ into three-dimensional space. We characterize the cuboid by $\mathcal{Q} = [u_0, u_1] \times [v_0, v_1] \times [w_0, w_1]$ and write $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v, w)$ with $(u, v, w) \in \mathcal{Q}$. We require that the Jacobian

$$J = \frac{\partial(\xi_1, \xi_2, \xi_3)}{\partial(u, v, w)} = \det \begin{pmatrix} \frac{\partial \xi_1}{\partial u} & \frac{\partial \xi_2}{\partial u} & \frac{\partial \xi_3}{\partial u} \\ \frac{\partial \xi_1}{\partial v} & \frac{\partial \xi_2}{\partial v} & \frac{\partial \xi_3}{\partial v} \\ \frac{\partial \xi_1}{\partial w} & \frac{\partial \xi_2}{\partial w} & \frac{\partial \xi_3}{\partial w} \end{pmatrix} \tag{A.35}$$

vanishes nowhere. Note that the rows in Eq. (A.35) are the three tangential vectors. They must be linearly independent which is expressed by $J \neq 0$.

The cuboid $\mathcal{Q}$ has a boundary $\partial\mathcal{Q}$ which is made up of eight differentiable pieces. Each piece shall be oriented such that the normal vector points outward. The surface $\partial\mathcal{Q}$ is mapped by $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v, w)$ to the surface $\partial\mathcal{V}$ of the volume which is closed.

As an example, let us study a ball $\mathcal{B}$ of radius R. We parameterize it by[4]

$$\boldsymbol{\xi}(r, \theta, \phi) = \begin{pmatrix} r \cos\theta \cos\phi \\ r \cos\theta \sin\phi \\ r \sin\theta \end{pmatrix}, \tag{A.36}$$

where $0 \leq r \leq R$, $-\pi/2 \leq \theta \leq \pi/2$ and $0 \leq \phi \leq 2\pi$.

The Jacobian is

$$\frac{\partial(\xi_1, \xi_2, \xi_3)}{\partial(r, \theta, \phi)} = r^2 \cos\theta. \tag{A.37}$$

It is singular at the center ($r = 0$) and on the earth axis ($\theta = \pm\pi/2$). We shall ignore this complication for the moment.

Let us discuss the six pieces of the surface.

- $r = 0$: the center, a point. Plays no role.
- $r = R$: the ball surface proper.
- $\theta = -\pi/2$: the south pole, a point. Does not contribute.
- $\theta = \pi/2$: the north pole. To be ignored.
- $\phi = 0$: a disk of radius R such that the poles and Greenwich are located at its boundary.
- $\phi = 2\pi$: the same as above, but with opposite orientation.

---

[4] Geographical coordinates.

The last two contributions cancel each other, and therefore the boundary $\partial\mathcal{B}$ is parameterized by $\boldsymbol{\eta}(\phi,\theta) = \boldsymbol{\xi}(R,\theta,\phi)$. Note that we have interchanged the arguments θ and ϕ. By this we achieve that the normal vector

$$\boldsymbol{n}(\theta,\phi) \propto \frac{\partial\boldsymbol{\eta}}{\partial\phi} \times \frac{\partial\boldsymbol{\eta}}{\partial\theta} = R^2\cos\theta \begin{pmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ \sin\theta \end{pmatrix} \tag{A.38}$$

points radially away from the ball. Compare with Eq. (A.36).

A.4 Integrating Fields

Fields, which live in three dimensional space and depend on time, can be integrated over one-, two-, or three-dimensional manifolds. We only discuss situations where these paths, surfaces and volumes are at rest, so that we may drop the time argument. The field integrals which we present here do not depend on the particular parameterization which we employ for calculating them. They are scalars. We also deal with generalizations of the fundamental theorem of calculus.

A.4.1 Path Integrals

We want to integrate a vector field $\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{x})$ along a path $\mathcal{C}$. Let $\boldsymbol{\xi} = \boldsymbol{\xi}(u)$ be a parameterization of the path, for $u_0 \le u \le u_1$. We consider two neighboring points $\boldsymbol{\xi}(u)$ and $\boldsymbol{\xi}(u + \mathrm{d}u)$. The vector transporting the first to the second point is

$$\mathrm{d}\boldsymbol{s} = \boldsymbol{\xi}(u+\mathrm{d}u) - \boldsymbol{\xi}(u) = \frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}u}\mathrm{d}u. \tag{A.39}$$

With this in mind we define

$$\int_{\mathcal{C}} \mathrm{d}\boldsymbol{s}\cdot\boldsymbol{V} = \int_{u_0}^{u_1} \mathrm{d}u\,\frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}u}\cdot\boldsymbol{V}(\boldsymbol{\xi}(u)). \tag{A.40}$$

The notation suggests that the integral depends on the path and on the vector field only, and this is so indeed.

Let us choose another parameterization $\bar{\boldsymbol{\xi}} = \bar{\boldsymbol{\xi}}(\bar{u}) = \boldsymbol{\xi}(u)$ of the same path $\mathcal{C}$. We calculate

$$\int_{\bar{u}_0}^{\bar{u}_1} \mathrm{d}\bar{u}\,\frac{\mathrm{d}\bar{\boldsymbol{\xi}}(\bar{u})}{\mathrm{d}\bar{u}}\cdot\boldsymbol{V}(\bar{\boldsymbol{\xi}}(\bar{u})) = \int_{u_0}^{u_1} \mathrm{d}u\,\frac{\mathrm{d}\bar{u}}{\mathrm{d}u}\frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}\bar{u}}\cdot\boldsymbol{V}(\boldsymbol{\xi}(u)), \tag{A.41}$$

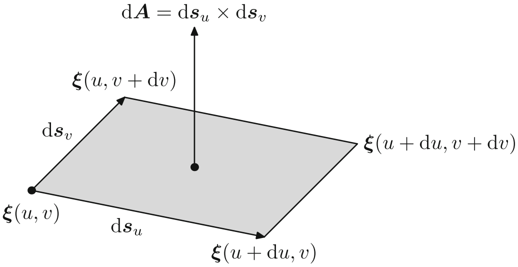

Fig. A.5 An infinitesimal surface element. The vectors $\mathbf{d}s_u$ and $\mathbf{d}s_v$ span a parallelogram. The vector product $\mathbf{d}s_u \times \mathbf{d}s_v$ is normal to the surface element, the modulus equals its area

and because of

$$\frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}\bar{u}} \frac{\mathrm{d}\bar{u}}{\mathrm{d}u} = \frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}u} \tag{A.42}$$

the integral (A.41) is the same as Eq. (A.40). For calculating the path integral one requires a particular parameterization, but any other parameterization will serve as well.

A.4.2 Surface Integrals

Let us parameterize a surface $\mathcal{A}$ by the mapping $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v)$ where $u \in [u_0, u_1]$ and $v \in [v_0, v_1]$. We concentrate on a typical surface element. This is spanned by vectors $\mathrm{d}\boldsymbol{s}_u = \boldsymbol{\xi}(u+\mathrm{d}u, v) - \boldsymbol{\xi}(u, v)$ and $\mathrm{d}\boldsymbol{s}_v = \boldsymbol{\xi}(u, v+\mathrm{d}v) - \boldsymbol{\xi}(u, v)$. Note $\mathrm{d}\boldsymbol{s}_u = \mathrm{d}u\, \partial\boldsymbol{\xi}/\partial u$ and $\mathrm{d}\boldsymbol{s}_v = \mathrm{d}v\, \partial\boldsymbol{\xi}/\partial v$ (Fig. A.5).

The vector product $\mathrm{d}\boldsymbol{A} = \mathrm{d}\boldsymbol{s}_u \times \mathrm{d}\boldsymbol{s}_v$ is a vector perpendicular to the surface element. Its modules is equal to the area of the surface element $\mathrm{d}\mathcal{A}$. This motivates us to define the surface integral of a vector field $\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{x})$ as

$$\int_{\mathcal{A}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{V} = \int_{u_0}^{u_1} \mathrm{d}u \int_{v_0}^{v_1} \mathrm{d}v \left(\frac{\partial\boldsymbol{\xi}(u, v)}{\partial u} \times \frac{\partial\boldsymbol{\xi}(u, v)}{\partial v} \right) \cdot \boldsymbol{V}(\boldsymbol{\xi}(u, v)). \tag{A.43}$$

The field is projected onto the normal of a surface element and multiplied by its area, and the integral is a "sum" over all surface elements.

The surface integral (A.44) does not depend on the particular parameterization which we employ to calculate it. We select another representation $\bar{\boldsymbol{\xi}}(\bar{u}, \bar{v}) = \boldsymbol{\xi}(u, v)$. Because of

$$\mathrm{d}\bar{u}\mathrm{d}\bar{v} = \mathrm{d}u\mathrm{d}v\, \frac{\partial(\bar{u}, \bar{v})}{\partial(u, v)} \tag{A.44}$$

and

$$\frac{\partial(\bar{u}, \bar{v})}{\partial(u, v)} \left(\frac{\bar{\boldsymbol{\xi}}(\bar{u}, \bar{v})}{\partial\bar{u}} \times \frac{\bar{\boldsymbol{\xi}}(\bar{u}, \bar{v})}{\partial\bar{v}} \right) = \frac{\partial\xi(u, v)}{\partial u} \times \frac{\partial\xi(u, v)}{\partial v} \tag{A.45}$$

we conclude

$$\int_{\bar{u}_0}^{\bar{u}_1} \mathrm{d}\bar{u} \int_{\bar{v}_0}^{\bar{v}_1} \mathrm{d}\bar{v} \left(\frac{\partial \bar{\boldsymbol{\xi}}(\bar{u},\bar{v})}{\partial \bar{u}} \times \frac{\partial \bar{\boldsymbol{\xi}}(\bar{u},\bar{v})}{\partial \bar{v}} \right) \cdot \boldsymbol{V}(\bar{\boldsymbol{\xi}}(\bar{u},\bar{v})) = \int_{\mathcal{A}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{V}. \tag{A.46}$$

Indeed, the surface integral is the same for all parameterizations.

As an example, let us work out the integral of $\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{x}/|\boldsymbol{x}|^3$ over a sphere $\mathcal{S}$ of radius R. We parameterize

$$\boldsymbol{\xi}(\theta,\phi) = R \begin{pmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ \sin\theta \end{pmatrix} = R\,\boldsymbol{n} \tag{A.47}$$

for $-\pi/2 \le \theta \le \pi/2$ and $0 \le \phi \le 2\pi$. With Eq. (A.38) one calculates

$$\mathrm{d}\boldsymbol{A} = R^2\,\mathrm{d}\theta\,\cos\theta\,\mathrm{d}\phi\,\boldsymbol{n} \tag{A.48}$$

and

$$\int_{\mathcal{S}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{V} = \int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, R^2 \cos\theta\, \frac{1}{R^2}\, \boldsymbol{n}\cdot\boldsymbol{n} = 4\pi. \tag{A.49}$$

A.4.3 Volume Integrals

We speak about a volume $\mathcal{V}$ which is parameterized by $\boldsymbol{\xi} = \boldsymbol{\xi}(u,v,w)$. The three vectors $\mathrm{d}\boldsymbol{s}_u = \boldsymbol{\xi}(u+\mathrm{d}u,v,w) - \boldsymbol{\xi}(u,v,w)$ and similarly $\mathrm{d}\boldsymbol{s}_v$ and $\mathrm{d}\boldsymbol{s}_w$ span an infinitesimal volume element. Its content is

$$\mathrm{d}V = (\boldsymbol{s}_u \times \boldsymbol{s}_v) \cdot \boldsymbol{s}_w = \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\, \frac{\partial(\xi_1,\xi_2,\xi_3)}{\partial(u,v,w)}. \tag{A.50}$$

See Eq. (A.35) for the definition of the Jacobian.

The volume integral of a scalar field $S = S(\boldsymbol{x})$ is given by

$$\int_{\mathcal{V}} \mathrm{d}V\, S = \int_{u_0}^{u_1} \mathrm{d}u \int_{v_0}^{v_1} \mathrm{d}v \int_{w_0}^{w_1} \mathrm{d}w\, \frac{\partial(\xi_1,\xi_2,\xi_3)}{\partial(u,v,w)}\, S(\boldsymbol{\xi}(u,v,w)). \tag{A.51}$$

Again, the volume integral does not change if calculated with another parameterization. With $\bar{\boldsymbol{\xi}}(\bar{u},\bar{v},\bar{w}) = \boldsymbol{\xi}(u,v,w)$ one finds

$$\mathrm{d}\bar{u}\,\mathrm{d}\bar{v}\,\mathrm{d}\bar{w}\, \frac{\partial(\bar{\xi}_1,\bar{\xi}_2,\bar{\xi}_3)}{\partial(\bar{u},\bar{v},\bar{w})} = \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\, \frac{\partial(\bar{u},\bar{v},\bar{w})}{\partial(u,v,w)}\, \frac{\partial(\xi_1,\xi_2,\xi_3)}{\partial(\bar{u},\bar{v},\bar{w})}. \tag{A.52}$$

The product of the Jacobians in Eq. (A.52) is $\partial(\xi_1, \xi_2, \xi_3)/\partial(u, v, w)$, and we arrive at

$$\int_{\bar{u}_0}^{\bar{u}_1} \mathrm{d}\bar{u} \int_{\bar{v}_0}^{\bar{v}_1} \mathrm{d}\bar{v} \int_{\bar{w}_0}^{\bar{w}_1} \mathrm{d}\bar{w} \, \frac{\partial(\bar{\xi}_1, \bar{\xi}_2, \bar{\xi}_3)}{\partial(\bar{u}, \bar{v}, \bar{w})} \, S(\bar{\boldsymbol{\xi}}(\bar{u}, \bar{v}, \bar{w})) = \int_{\mathcal{V}} \mathrm{d}V \, S. \tag{A.53}$$

The volume element for spherical coordinates Eq. (A.36) reads

$$\mathrm{d}V = \mathrm{d}r \, \mathrm{d}\theta \, \mathrm{d}\phi \, r \cos\theta. \tag{A.54}$$

A.4.4 Stokes' and Gauss' Theorems

The fundamental theorem of calculus reads

$$\int_a^b dx \, f'(x) = f(b) - f(a), \tag{A.55}$$

where $f = f(x)$ is a differentiable function on $[a, b]$. There are generalizations for one-, two- and three-dimensional manifolds.

The Gradient Theorem

Consider a path $\mathcal{C}$ and a scalar field S with gradient ∇S. Let $\boldsymbol{\xi} = \boldsymbol{\xi}(u)$ be a parameterization. We calculate

$$\int_{u_0}^{u_1} \mathrm{d}u \, \frac{\mathrm{d}\boldsymbol{\xi}(u)}{\mathrm{d}u} \cdot \nabla S(\boldsymbol{\xi}(u)) = \int_{u_0}^{u_1} \mathrm{d}u \, \frac{\mathrm{d}S(\xi(u))}{\mathrm{d}u} = S(\boldsymbol{x}_1) - S(\boldsymbol{x}_0). \tag{A.56}$$

The left hand side is a path integral which does not depend on the particular parameterization, and the same applies to the right-hand side. Recall that $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ are the starting and the end points of the path, respectively. Hence we may write

$$\int_{\mathcal{C}} \mathrm{d}\boldsymbol{s} \cdot \nabla S = S(\boldsymbol{x}_1) - S(\boldsymbol{x}_0). \tag{A.57}$$

The similarity with Eq. (A.55) is obvious.

The Curl, or Stokes' Theorem

Consider a surface $\mathcal{A}$ and a vector field $\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{x})$. The boundary $\partial\mathcal{A} = \partial\mathcal{A}_1 + \partial\mathcal{A}_2 + \partial\mathcal{A}_3 + \partial\mathcal{A}_4$ consists of four smooth pieces which we have enumerated as shown in Fig. A.3.

Stokes' theorem says

$$\int_{\mathcal{A}} \mathrm{d}\boldsymbol{A} \cdot (\boldsymbol{\nabla} \times \boldsymbol{V}) = \int_{\partial\mathcal{A}} \mathrm{d}\boldsymbol{s} \cdot \boldsymbol{V}. \tag{A.58}$$

The proof of this curl theorem is similar to that of the gradient theorem, but not quite as simple.

We choose a parameterization $\boldsymbol{\xi} = \boldsymbol{\xi}(u, v)$ and integrate over $u \in [u_0, u_1]$ and $v \in [v_0, v_1]$.

The integrand is[5]

$$\epsilon_{ijk}\epsilon_{ilm}\frac{\partial\xi_j}{\partial u}\frac{\partial\xi_k}{\partial v}\,\partial_l V_m(\boldsymbol{\xi}). \tag{A.59}$$

The two epsilons contract to

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{kl}\delta_{jm} - \delta_{km}\delta_{jl}, \tag{A.60}$$

giving rise to

$$\frac{\partial\xi_j}{\partial v}\frac{\partial\xi_k}{\partial v}\,\partial_k V_j - \frac{\partial\xi_k}{\partial u}\frac{\partial\xi_j}{\partial v}\,\partial_j V_k. \tag{A.61}$$

This may be rewritten as

$$\frac{\partial\xi_k}{\partial v}\frac{\partial V_k}{\partial u} - \frac{\partial\xi_k}{\partial u}\frac{\partial V_k}{\partial v}. \tag{A.62}$$

The first contribution equals

$$\frac{\partial}{\partial u}\frac{\partial\xi_k}{\partial v}\,V_k - V_k\,\frac{\partial^2\xi_k}{\partial u\partial v}, \tag{A.63}$$

the second reads

$$-\frac{\partial}{\partial v}\frac{\partial\xi_k}{\partial u}\,V_k + V_k\,\frac{\partial^2\xi_k}{\partial v\partial u}. \tag{A.64}$$

Two terms drop out, and we are left with

$$\int_{u_0}^{u_1}\mathrm{d}u\int_{v_0}^{v_1}\mathrm{d}v\,\left(\frac{\partial}{\partial u}\frac{\partial\boldsymbol{\xi}}{\partial v}\cdot\boldsymbol{V}(\boldsymbol{\xi}) - \frac{\partial}{\partial v}\frac{\partial\boldsymbol{\xi}}{\partial u}\cdot\boldsymbol{V}(\boldsymbol{\xi})\right) \tag{A.65}$$

for the left hand side of Eq. (A.58). Integrating the first term over u yields two boundary terms, and another two contributions come from integrating the second term over v. They are

$$\int_{v_0}^{v_1}\mathrm{d}v\,\frac{\partial\boldsymbol{\xi}(u_1, v)}{\partial v}\cdot\boldsymbol{V}(\boldsymbol{\xi}(u_1, v)) \tag{A.66}$$

---

[5] Einstein's summation convention.

and

$$-\int_{v_0}^{v_1} \mathrm{d}v \, \frac{\partial \boldsymbol{\xi}(u_0, v)}{\partial v} \cdot \boldsymbol{V}(\boldsymbol{\xi}(u_0, v)). \tag{A.67}$$

These are path integrals of $\boldsymbol{V}$ over $\partial\mathcal{A}_2$ and $\partial\mathcal{A}_4$ with proper signs (see Fig. A.3). Integrating the second term in Eq. (A.65) yields the remaining path integrals. We have thus proven Stokes' theorem.

The Divergence, or Gauss' Theorem

Assume a volume $\mathcal{V}$ and a v field $\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{x})$. The divergence, or Gauss' theorem reads

$$\int_{\mathcal{V}} \mathrm{d}V \, \nabla \cdot \boldsymbol{V} = \int_{\partial\mathcal{V}} \mathrm{d}\boldsymbol{A} \cdot \boldsymbol{V}. \tag{A.68}$$

The proof is similar to the proof of Stokes' theorem, although it requires a lot of bookkeeping. We will not present it here.

The result is rather plausible. The integral of a field derivative over a manifold coincides with the integral of the field over a manifold with one dimension less. For a surface the field and the field derivative must be vectors, i.e., a vector field and its curl. For a volume the field must be a vector and the field derivative a scalar, i.e., the divergence of a vector field.

A.5 More on Fields

We have mentioned already that the time derivative of a scalar field does *not* behave as a scalar field under Galilei transformations. Therefore, time derivatives must always be accompanied by expression which compensate for this. We shall discuss the transformation properties of balance equations and justify why the conduction contribution to currents transforms as a vector field.

A.5.1 Densities and Current Densities

Denote by $\nu = 1, 2, \dots$ the particles of a certain species. Its density is

$$n(t, \boldsymbol{x}) = \sum_{\nu} \langle \, \delta^3(\boldsymbol{x} - \boldsymbol{x}_\nu(t)) \, \rangle. \tag{A.69}$$

$\boldsymbol{x}_\nu(t)$ is the observable "location of particle ν at time t" in the Heisenberg picture and $\langle \dots \rangle$ denotes the expectation value of the (local) Gibbs state.

If $(t',\boldsymbol{x}')$ and $(t,\boldsymbol{x})$ are related by a Galilei transformation

$$t = t' + \tau \text{ and } \boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t', \tag{A.70}$$

we easily show

$$n(t,\boldsymbol{x}) = n'(t',\boldsymbol{x}'), \tag{A.71}$$

because of $\delta^3(z) = \delta^3(Rz)$. Recall that R is an orthogonal matrix.

Thus, particle densities transform as scalar fields, and the same applies to the mass density

$$\varrho(M;t,\boldsymbol{x}) = \sum_a m_a n_a(t,\boldsymbol{x}). \tag{A.72}$$

$a = 1, 2, \dots$ enumerates the particle species, and m_a is the mass of a particle of species a.

The particle current density belonging to Eq. (A.69) is

$$\boldsymbol{j}(t,\boldsymbol{x}) = \sum_\nu \langle\, \dot{\boldsymbol{x}}_\nu \, \delta^3(\boldsymbol{x} - \boldsymbol{x}_\nu(t))\, \rangle. \tag{A.73}$$

It transforms as

$$\boldsymbol{j}(t,\boldsymbol{x}) = R\boldsymbol{j}'(t',\boldsymbol{x}') + n(t',\boldsymbol{x}')\,\boldsymbol{u}. \tag{A.74}$$

The particle current density does *not* transform as a vector field, and the same is true for the mass current density

$$\boldsymbol{j}(M;t,\boldsymbol{x}) = \sum_a m_a \boldsymbol{j}_a(t,\boldsymbol{x}) \tag{A.75}$$

for which we find

$$\boldsymbol{j}(M;t,\boldsymbol{x}) = R\boldsymbol{j}'(M;t',\boldsymbol{x}') + \varrho(M;t',\boldsymbol{x}')\,\boldsymbol{u}. \tag{A.76}$$

Recall that the local center of mass velocity field $\boldsymbol{v} = \boldsymbol{v}(t,\boldsymbol{x})$ is the mass current density divided by the mass density. With respect to the Galilei group it transforms as

$$\boldsymbol{v}(t,\boldsymbol{x}) = R\,\boldsymbol{v}'(t',\boldsymbol{x}') + \boldsymbol{u}. \tag{A.77}$$

This is highly plausible.

There is nothing particular about the particle current density and its transformation behavior (A.75). Any current density transforms in this way,

$$\boldsymbol{j}(Y;t,\boldsymbol{x}) = R\boldsymbol{j}'(Y;t',\boldsymbol{x}') + \varrho(Y;t',\boldsymbol{x}')\,\boldsymbol{u}. \tag{A.78}$$

We conclude that the conduction current density

$$\boldsymbol{J}(Y;t,\boldsymbol{x}) = \boldsymbol{j}(Y;t,\boldsymbol{x}) - \varrho(Y;t,\boldsymbol{x})\,\boldsymbol{v}(t,\boldsymbol{x}) \tag{A.79}$$

transforms properly as a vector field.

A.5.2 Time Derivatives

Let us work out the transformation behavior of $\dot{\varrho} + \partial_i \varrho v_i$ for a physical quantity Y which we do not write explicitly. We calculate

$$\partial_{t'} \varrho' + \partial_i' \varrho' v_i' = \partial_t \varrho + u_i \partial_i \varrho + \partial_i \varrho v_i - u_i \partial_i \varrho. \tag{A.80}$$

$RR^\dagger$ has already been worked in. We conclude that expression $\dot{\varrho}(Y) + \partial_i \varrho(Y) v_i$ is a scalar field, just as $\partial_i J_i(Y)$. It follows from the prototype balance equation that volumetric production rates $\pi(Y)$ are scalar fields as well. We have used these findings before, see subsection *Transformation properties of currents* in Chap. 1.

What about $\mathrm{D}_t = \partial_t + \boldsymbol{v} \cdot \boldsymbol{\nabla}$, the substantial time derivative?

For an arbitrary scalar field S we write

$$\mathrm{D}_{t'} S' = \partial_t S + u_i \partial_i S + v_i \partial_i S - u_i \partial_i S. \tag{A.81}$$

If follows that the substantial time derivative operator D_t transforms as a scalar under Galilei transformations.

Glossary

The entries in this list of key words and persons are ordered alphabetically. ▹ is a hint to another glossary entry. Persons are briefly described by their origin, field of activity, and life span. The association British, English, Irish or Scottish is somewhat arbitrary. Likewise, the distinction between natural science, philosophy, mathematics, astronomy, physics, chemistry and engineering is less clear for earlier centuries.

A

Airy, George: English astronomer and mathematician, 1801–1892. Mentioned in article *Stress Concentration*.

Ampère, André-Marie: French physicist, 1775–1836.

Ångström, Anders Jonas: Swedish physicist, 1814–1874.

Archimedes, of Syracuse: Greek mathematician, physicist, engineer, inventor, and astronomer, 285–212 BC.

Archimedes' principle The buoyancy force of a partially or totally immersed body is equal to the weight of the displaced fluid. Although strictly valid only for an ▹ *incompressible* fluid, the corrections for compressible media, like an ▹ *ideal gas*, are tiny. Read the corresponding article.

Avogadro, Amadeo: Italian physicist, 1776–1856.

Avogadro's number One mole of the C^{12} isotope weighs 12 g, by definition. This mass consists of N_A atoms, a number which is known as Avogadro's or ▹ *Loschmidt's number*. Avogadro's number N_A=6.022141×10^{23} links continuum physics to microphysics. For example, ▹ *Boltzmann's constant* k_B and the ▹ *universal gas constant* R are related by $R = N_A k_B$.

P. Hertel, *Continuum Physics*, Graduate Texts in Physics,
DOI 10.1007/978-3-642-29500-3,

B

Bach, Johann Sebastian: German musical composer, 1685–1770. Mentioned in article *Vibrating Strings and Membranes*.

Balance equation Balance equations state that a ▹ *quantity* Y within a certain region of space, or volume, may change in the course of time because of inflow via the surface or production within. This is expressed by the balance equation $\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y)$. Here $\varrho(Y), \boldsymbol{j}(Y)$ and $\pi(Y)$ are the ▹ *density*, ▹ *current density* and ▹ *volumetric production rate* of quantity Y, respectively. Read section *Densities for Content, Flow and Production Rate* for their definition and section *More on Fields* for transformation properties.

Beam bending A beam, if not strained, is a long straight column of constant cross section. It serves to guide momentum, i.e., transmit forces. The partial differential equations of elasticity theory simplify considerably if fields are approximated linearly with respect to cross section coordinates. There is a neutral fiber ($x = y = 0$ and $0 \le z \le \ell$) the displacement of which is described by $X(z)$ and $Y(z)$. Both displacements obey ordinary differential equation of fourth order, the solutions of which are governed by transversal loads, longitudinal stress or pressure, and boundary conditions. Beams tend to buckle if the pressure on the top face exceeds a certain limit, ▹ *Euler instability*. Read article *Beam Bending and Buckling*.

Bernoulli, Jakob: Swiss mathematician and physicist, 1645–1705. Mentioned in articles *Beam Bending and Buckling and Bernoulli's Law*.

Boltzmann, Ludwig: Austrian physicist, 1844–1906.

Boltzmann constant Introduced by Max Planck who recognized that the entropy of thermodynamics and the logarithm of the micro-canonical sum of states are proportional. In this book, we have introduced k_B by $S(W) = -k_B \operatorname{tr} W \ln W$, where W describes the mixed state and $S(W)$ its entropy. Today's rather accurate value k_B=$1.380649 \times 10^{-23}\,\mathrm{J\,K^{-1}}$results from an accurate determination of ▹ *Avogadro's number* by particle counting. Earlier less precise values came from fluctuation measurements (▹ *Johnson noise*, ▹ *Nyquist formula*, and ▹ *Brownian motion*).

Brown, Robert: Scottish botanist, 1773–1858.

Brownian motion A particle which is just large enough to be seen in a microscope moves seemingly at random if suspended in a liquid. ▹ *Einstein* was the first to propose that it is the thermally agitated environment which kicks the particle. Moreover, he could work out the root mean square displacement as a function of time. This discovery allowed to measure the ▹ *Boltzmann constant*, or, equivalently, ▹ *Avogadro's number*. We not only present Einstein's original reasoning, but also solve the ▹ *Langevin equation* for the motion of a particle with friction driven by a random force of constant spectral density, or ▹ *white noise*. Brownian motion is the diffusion of a single particle, or, put otherwise, diffusion is mass-wise Brownian motion. Read the corresponding article.

Buckling Long thin beams tend to buckle if they have to stand too large an axial force. ▹ *Euler instability*.

C

Chandrasekhar, Subrahmanyan: Indian/US-American astrophysicist, 1910–1995.

Chandrasekhar's limit The mass of a ▹ *white dwarf* must not exceed 1.44 sun masses. White dwarfs with sub-critical mass which suck up matter from a companion star will explode if Chandrasekhar's limit is reached. The corresponding Ia supernova serves as a standard candle, it allows to measure the distance of far away objects. More in article *White Dwarfs*.

Chemical potential A physical system is always a subsystem within its environment. If particles of species a are allowed to cross the boundary of the system, in and out, equilibrium is characterized by equal chemical potential μ_a inside and outside. Read section *Statistical Thermodynamics*. Gradients of a chemical potential cause diffusion. ▹ *Electrochemical potential*.

Chemical reaction In a chemical reaction, which is assumed to occur instantaneously, particles of certain species vanish and other particles appear. In one reaction of type r, ν^{ra} particles of species a are created. A negative value indicates disappearance. The ν^{ra} are ▹ *stoichiometric coefficients*, they have no common divisor. Let Γ^r denotes the number of reactions of type r per unit volume and per unit time. The volumetric production rate of a-particles is given by $\pi(N^a) = \sum_r \Gamma^r \nu^{ra}$.

Compression modulus An elastic body subject to hydrostatic pressure p experiences a relative volume change p/K. The compression modulus is given by $K = E/3(1-2\nu)$ where E and ν are ▹ *Young's modulus* and ▹ *Poisson's ratio*, respectively. Read article *Elasticity Moduli*.

Conduction Transport of a quantity Y by interaction, not ▹ *convection*. Examples are diffusion of particles, of phonons (heat conduction) and the elastic or inelastic transport of momentum as described by the stress tensor. ▹ *Current density*. Read section *Convection and Conduction*.

Conductivity ▹ *Ohm's law* for electric conductivity. Conductivities in a wider sense are defined as follows. Denote by $\lambda_1, \lambda_2 \dots$ the external parameters (forces) of a system and by $V_r = -\langle\, \partial H/\partial\lambda_r \,\rangle$ the corresponding reactions, such that the work done on a system is $\mathrm{d}A = -\sum_r V_r \,\mathrm{d}\lambda_r$. Denote by $\Phi_r = \dot{V}_r$ the rate of change, or flux. For oscillating forces one obtains, in linear approximation, a linear relationship $\tilde{\Phi}_r = \sum_s K_{rs}\tilde{\lambda}_r$ between fluxes and forces (the tilde denotes the Fourier transform). The proportionality constants $K_{rs} = K_{rs}(\omega)$ are generalized conductivities. This matrix fulfills ▹ *Onsager's relations*. Interchanging the indexes r and s as well as inverting a quasi-static magnetic field is a symmetry.

Convection If matter flows, its material points transport their properties Y from one place to another. The corresponding current density is $\varrho(Y)\,\boldsymbol{v}$, where $\boldsymbol{v}$ is the center of mass flow velocity. ▹ *Current density*. Read section *Convection and Conduction*.

Current density The current of quantity Y through a surface element $\mathrm{d}\boldsymbol{A}$ is given by $\mathrm{d}I(Y) = \boldsymbol{j}(Y) \cdot \mathrm{d}\boldsymbol{A}$. Its physical dimension is [Y] per second per square meter. Current densities are classified as convective (the quantity is transported together with mass by flowing) or conductive (transported by interactions). The former is given by $\varrho(Y)\,\boldsymbol{v}$, the latter is the rest $\boldsymbol{J}(Y) = \boldsymbol{j}(Y) - \varrho(Y)\,\boldsymbol{v}$. The conduction current density, in turn, may be split into an elastic (reversible) and an inelastic (irreversible) contribution, $\boldsymbol{J}'(Y)$ and $\boldsymbol{J}''(Y)$, respectively; they behave oppositely upon time reversal. Only conduction currents transform properly as ▹ *vectors* and may be associated with other vector fields by ▹ *material equations*.

Curve ▹ *Path.*

D

Degeneracy pressure There are two sorts of particles. ▹ *Fermions* want to be alone, ▹ *bosons* like other particles close by. Fermions, in particular electrons, cannot occupy the same state more than once (▹ *Pauli exclusion principle*), they are degenerate. The pressure $p = p(T, n)$ of non-interacting fermions obeys the ideal gas formula for very small particle density n. In particular, it vanishes with $T \to 0$. For large n, however, there is a degeneracy pressure proportional to $n^{5/3}$ even for zero temperature. This pressure stabilizes a ▹ *white dwarf* which consist of a plasma of carbon and oxygen nuclei and electrons. Read article *White Dwarfs* for the material equation of a dense gas of non-interacting fermions.

Density A ▹ *quantity* Y is an additive and transportable property of a system. The content of Y in a volume $\mathcal{V}$ may therefore by written as a volume integral over a density field $\varrho(Y) = \varrho(Y; t, \boldsymbol{x})$. The physical dimension of $\varrho(Y)$ is [Y] per cubic meter. Density in this book is practically always quantity per unit volume, although in some situations we speak of a surface charge density or of the density of states, and so forth. ▹ *Balance equation*.

Descartes, René (Cartesius): French philosopher and mathematician, 1596–1650.

Dielectric permittivity ▹ *Dielectric susceptibility*.

Dielectric susceptibility An oscillating electric field strength $\tilde{E}_j(\omega)$ produces a polarization $\tilde{P}_i(\omega)$ which is, in linear approximation, proportional to it. The proportionality factor in $\tilde{P}_i(\omega) = \epsilon_0 \chi_{ij} \tilde{E}_i(\omega)$ defines the dielectric susceptibility $\chi_{ij} = \chi_{ij}(\omega)$. The properties of it are thoroughly studied in Chap. 3. Recall that the dielectric displacement is $\tilde{D}_i = \epsilon_0 E_i + \tilde{P}_i = \epsilon_0 \epsilon_{ij} \tilde{E}_j$. Therefore the (relative) dielectric permittivity is given by $\epsilon_{ij}(\omega) = \delta_{ij} + \chi_{ij}(\omega)$.

Dielectric waveguide A device which guides light within a region of increased dielectric permittivity. A planar waveguide is characterized by a profile $\epsilon = \epsilon(x)$, a linear waveguide by $\epsilon = \epsilon(x, y)$. Modes are solutions of Maxwell's equations of the form $F(t, \boldsymbol{x}) = f(x) \exp(\mathrm{i}\beta z) \exp(-\mathrm{i}\omega t)$ for planar waveguides and with $f = f(x, y)$ for linear waveguides. For given angular frequency ω, only some discrete propagation constants $\beta_1, \beta_2, \dots$ are allowed. Read the article *Planar Dielectric Waveguides* and *Surface Plasmon Polaritons*.

Diffusion constant The current density for ▷ *particles* of species a is given by $\boldsymbol{j}(N^a) = n^a \boldsymbol{v} + \boldsymbol{J}^a$, where n^a denotes the particle density and $\boldsymbol{v}$ is the center of mass flow velocity. The ▷ *conduction* part $\boldsymbol{J}^a$ is proportional to the driving force, usually the gradient of the chemical potential μ^a. For constant temperature, the chemical potential depends on location via the particle density, therefore $\boldsymbol{J}^a = -D\nabla n^a$ is a plausible material equation (Fick's law). The diffusion constant D cannot be negative, according to the ▷ *second main law* of thermodynamics. Read section *Diffusion* of Chap. 2.

Diffusion equation If particles are suspended in a medium at rest, they tend to diffuse until a spatially constant distribution is attained. The particle density $n = n(t, \boldsymbol{x})$ obeys $\dot{n} = D\,\Delta n$, the diffusion equations. ▷ *Fick's law*. Read section *Diffusion* of Chap. 2. Diffusion combined with chemical reactions may produce interesting effects, such as pattern formation. ▷ *Reaction-diffusion*.

Dispersion relation A causal function f obeys $f(t) = \theta(t) f(t)$, where θ is Heaviside's step function. The Fourier transform $\tilde{f}$ consequently is a convolution of $\tilde{f}$ itself and the Fourier transform of the step function. The resulting relation describes dispersion, because $\tilde{f} = \tilde{f}(\omega)$ necessarily depends on ω. The real, or refractive part, is an integral over the imaginary, or absorptive part. There is no refraction without absorption. ▷ *Kramers-Kronig relations* which specialize this to the field of optics. Read the corresponding section of Chap. 3. Also ▷ *Sellmeier formula*.

Drude, Paul: German physicist, 1863–1906.

Drude model In a solid, a typical electron is bound to an ion. Its deviation $\boldsymbol{x}$ from the equilibrium position is influenced by external electric and magnetic fields according to $m(\ddot{\boldsymbol{x}} + \Gamma\dot{\boldsymbol{x}} + \Omega^2\boldsymbol{x}) = -e\{\boldsymbol{E} + \dot{\boldsymbol{x}} \times \boldsymbol{B}\}$. Γ describes friction, $m\Omega^2$ is the spring constant, $\boldsymbol{E}$ and $\boldsymbol{B}$ are the electric field strength and magnetic induction, respectively. The Drude model provides rough estimates for the ▷ *dielectric susceptibility*, the ▷ *electric conductivity*, the ▷ *Hall effect* and the ▷ *Faraday effect*.

E

Einstein, Albert: German physicist, 1879–1955. Mentioned in article *Brownian Movement*.

Einstein summation convention If in an expression an index referring to space directions occurs twice, a sum over it is automatically understood. Thus the divergence of a vector field $\boldsymbol{V}$, namely $\nabla \cdot \boldsymbol{V}$ or $\partial_1 V_1 + \partial_2 V_2 + \partial_3 V_3$ reads $\partial_k V_k$ with Einstein's summation convention. The index k is dummy, it may be replaced by any other symbol not yet in use. An expression in this context is a product of tensors.

Electrochemical potential Mobile Electrons migrate because of two different reasons. They are either dragged by an electric field, the negative gradient of the electrical potential, or by a varying chemical potential μ^* of mobile electrons. The sum $\phi^e - \mu^*/e$ is the electrochemical potential. Its negative gradient drives the irreversible electric current density. Some authors also refer to $\bar{\mu}^* = \mu^* - e\phi^e$ as electrochemical potential. Read sections *Charge Transport and Ohm's Law and Hall Effect*.

Energy In quantum theory, the waiting operator is as $U_t = \exp(-\mathrm{i}tH/\hbar)$. t denotes ▹ *time* and H, the Hamilton operator, is the system's energy. For an autonomous system, it is conserved: its expectation value does not depend on time. In continuum physics, it is split into kinetic, potential and ▹ *internal* energy which are additive transportable quantities. Read section *Statistical Thermodynamics* as well as *Energy and the First Law of Thermodynamics*.

Entropy A ▹ *mixed state* is described by a probability matrix W. There is a complete set $\phi_1, \phi_2, \dots$ of pure states which occur with probabilities $w_1, w_2, \dots$ How much a state is mixed is described by it entropy $S(W) = -k_B \sum_i w_i \ln w_i$. The entropy of a pure state vanishes, it is positive otherwise. Mixing two mixed states increases the entropy. Read section *Statistical Thermodynamics*. Also ▹ *Boltzmann's constant*.

Euler, Leonhard: Swiss mathematician and physicist, 1707–1783.

External parameter A physical system is always embedded in its environment. Changes in the system influence the environment, and changes in the environment are felt by the system. However, there are situations where the influences of the environment, described by parameters $\lambda_1, \lambda_2, \dots$ cause changes in the system the influence of which on the environment may safely be neglected. Put otherwise, the feedback vanishes or is made to vanish. Such parameters, as the voltage of a power supply, the volume within which a fluid is confined, or the gravitational action of the earth on a small piece of matter, are called external parameters. The Hamiltonian $H = H(\lambda_1, \lambda_2, \dots)$ of the system may depend on such external parameters. They appear as parameters to be adjusted at will or given.

F

Faraday, Michael: English physicist, 1791–1867.

Faraday effect An external or internal quasi-static magnetic field affects the propagation of light. A linearly polarized beam propagating in field direction splits into circularly polarized beams with slightly differing refractive indexes. When leaving the probe, the beam is again linearly polarized. However, the polarization vector has been rotated by an angle which is proportional to the sample thickness. The proportionality factor, the ▹ *specific* Faraday rotation, can be estimated with the aid of the ▹ *Drude model*. If the reflected light beam passes through the same probe in backward direction, the rotation is *not* undone, but continues. The Faraday effect is non-reciprocal, as contrasted with ▹ *optical activity*. Read the corresponding article.

Fermi, Enrico: Italian/US-American physicist, 1901–1954.

Fick's law The diffusion current density is proportional to the particle density gradient, i.e., $\boldsymbol{J} = -D\nabla n$. The diffusion constant D is positive.

First main law The energy of a system can be classified as kinetic, potential, or internal. Kinetic and potential energy can be transformed away by choosing an appropriate system of reference. The Hamiltonian H then describes internal energy $U = \langle H \rangle = \operatorname{tr} WH$, where W is the system's state. This bilinear expression says $\mathrm{d}U = \operatorname{tr} \mathrm{d}WH + \operatorname{tr} W\mathrm{d}H$, or $\mathrm{d}U = \mathrm{d}Q + \mathrm{d}A$. The internal energy of a system may change because of heat or work. The former is brought about by a change of the system's state, the latter by an infinitesimal change of the external parameters of the Hamiltonian, $\mathrm{d}H(\lambda) = -\Lambda_r\, \mathrm{d}\lambda_r$. Within the framework of continuum physics, the substantial change of internal energy $\varrho\, \mathrm{D}_t\, u$ is made up of five terms. $T'_{ik} G_{ik}$ describes compression work, $J^{\mathrm{e}\,\prime}_i E_i$ is the work done to polarize a medium, $-\partial_i J^{\mathrm{u}}_i$ is the net heat inflow, $T''_{ik} G_{ik}$ the friction heat, and $J^{\mathrm{e}\,\prime\prime}_i E_i$ is Joule's heat. Read section *Energy and the First Law of Thermodynamics*.

Fluid A fluid, or a fluid medium, is characterized by the absence of shear stress if at rest or moving with constant velocity. The elastic part T'_{ik} of the stress tensor does not have non-diagonal entries. In fact, it is proportional to the unit tensor multiplied by $-p$, where p denotes the ▹ *pressure* field. One distinguishes between gases and liquids, the former being highly compressible, the latter nearly ▹ *incompressible*. Air under normal conditions is a prototype of a gas. Water under normal conditions is the prototype of an incompressible liquid. However, there is a continuous transition from liquid to gas when temperature and pressure are changed. Read section *Fluid Media* of Chap. 2.

Fourier, Joseph: French mathematician and physicist, 1768–1830.

Fourier's law The conduction part of the ▹ *internal energy* (heat) current density is proportional to the temperature gradient, i.e., $J^{\mathrm{u}}_i = -\lambda\, \partial_i T$. The proportionality factor λ is the ▹ *thermal conductivity* of the material. ▹ *Heat equation*.

Fowler, Ralph: British physicist, 1889–1944. Mentioned in article *White dwarfs*.

Free energy Introduced as a Lagrange parameter, the free energy F depends on ▹ *temperature* and the ▹ *external parameters* of the system. It is well defined for a system in its equilibrium, or ▹ *Gibbs* state. The free energy serves as a thermodynamic potential: to each variable there is a conjugate property which is calculated as a partial derivative. For example, $\partial F(T, V, \dots)/\partial V = -p(T, V, \dots)$ for volume V and ▹ *pressure* p. Read section *Statistical Thermodynamics*.

G

Galilei transformation If $(t, \boldsymbol{x})$ are time-space coordinates with respect to an ▹ *inertial frame of reference* Σ, then Σ' with coordinates $(t', \boldsymbol{x}')$ is likewise an inertial frame if new and old coordinates are related by a Galilei transformation

$t = t' + \tau$ and $\boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'$. R is an orthogonal matrix. The Galilei group consists of all transformations $\Gamma = \{\tau, \boldsymbol{a}, R, \boldsymbol{u}\}$.

Galileo, Galilei: Italian astronomer, mathematician and physicist, 1564–1642.

Gibbs, J. Willard: US-American physicist and chemist, 1839–1903.

Gibbs state The Gibbs state describes a system in thermal equilibrium. Among all ▹ *mixed states* W of a system with a given ▹ *internal energy* U, the Gibbs state G is maximally mixed, i.e., has the largest ▹ *entropy* $S(G) \geq S(W)$. The Gibbs state depends on ▹ *temperature* T and ▹ *external parameters*. If the system is open not only to energy, but also to particle exchange with the environment, the Gibbs state will also depend on ▹ *chemical potentials*. Read section *Statistical Thermodynamics* of Chap. 3.

Goodyear, Charles: US-American inventor, 1800–1860. Mentioned in article *Elasticity Moduli*.

Gray-Scott model A model with two species of particles U and V which mimics an auto-catalytic reaction U+2V→3V. New U particles enter the reactor via a membrane, and V particles pass outside through the same membrane. The particles are allowed to diffuse. In certain regions, the solution depends critically on the model parameters and gives rise to different kinds of regular patters which are either stable or oscillate. Read article *Reactions and Diffusion*.

Guided optical mode A packet of electromagnetic waves in a homogeneous medium may be focused, but finally spreads out in space. The medium must be inhomogeneous if microwaves or light waves are to be concentrated in a narrow region. Confining light in metallic tubes leads to unacceptably high losses by ▹ *Joule's heat*. Instead, a region of increased dielectric permittivity may confine the wave, or guide it. ▹ *Dielectric waveguides*. However, only discrete modes may propagate in planar or linear waveguides. If the waveguide is much broader than high, the modes are either ▹ *transversal electric or magnetic*. An optical TM mode can also be guided along the interface of a dielectric and a conducting medium with negative permittivity. ▹ *Surface plasmon polaritons*.

H

Hagen, Gotthilf: German physicist and hydraulic engineer, 1797–1884.

Hagen-Poiseuille law A circular pipe of length L and inner diameter $2R$ transports an amount of liquid per unit time given by $\dot{V} = \pi R^4 p'/8\eta$. Here $p' = \Delta p/L$ is the pressure decrease per unit length and η the viscosity. This formula was derived independently by ▹ *Hagen* and ▹ *Poiseuille*. It is valid for small ▹ *Reynold numbers* only, i.e., for laminar, not turbulent flow. Read the corresponding article.

Hall, Edwin: US-American physicist, 1855–1938.

Hall effect Assume an electric current density $\tilde{J}^{\mathrm{e}}_x$ in x-direction and a static magnetic induction $\mathcal{B}_y$ in y-direction. There will be an electric field strength

$\tilde{E}_z = R_H \tilde{J}^e_x \mathcal{B}_y$ in z-direction. This is true if boundary conditions prohibit a current in z-direction, a current which is stopped by $\tilde{E}_z$. The Hall constant $R_H = R_H(\omega)$ depends on the angular frequency of the AC current $\tilde{J}^e$, its sign indicates whether electrons or holes are the principal charge carriers. See article *Ohm's Law* and *Hall Effect* for details.

Heat equation If the ▹ *specific* ▹ *internal energy* depends on location only via its dependency on temperature T, an equation $\dot{T} = \kappa \Delta T$ can be derived. $\kappa = \lambda/\varrho c$ is called the thermal diffusivity of the material. ▹ *Fourier's* law for the definition of thermal conductivity λ. ϱ is the mass density and c denotes the specific heat capacity. Read section *Heat conduction* of Chap. 2.

Heisenberg picture ▹ *Time*.

Heisenberg, Werner: German physicist, 1901–1976.

Hooke, Robert: British mathematician and physicist, 1635–1703.

Hooke's law Strain, by definition, vanishes in an unstressed, relaxed elastic body. Therefore, it is a plausible assumption that ▹ *strain* depends linearly on ▹ *stress*, an assumption which can be traced back to Robert Hooke. Usually, before the stress-strain relation becomes nonlinear, the medium ceases to be elastic, it is deformed irreversibly or it brakes, often because of defects (read article *Stress Concentration*). In a crystalline medium with very low symmetry, the linear relation between strain and stress may contain as many as 21 formally independent elasticity constants. For isotropic media, cubic or amorphous, there are just two independent elasticity constants of which there are various combinations. ▹ *Young's modulus*, ▹ *Poisson's ratio*, ▹ *compression modulus*, ▹ *shear modulus*, ▹ *Lamé constants*.

I

Ideal gas If N particles are confined within a volume V the boundary of which has temperature T, the pressure at low particle density is given by $p = Nk_BT/V$. With $\nu = N/N_A$ as the number of moles, one may also write $p = \nu RT/V$. R is the ▹ *universal gas constant* and N_A represents ▹ *Avogadro's number*. All gases at low enough pressure behave the same with respect to pressure. The heat capacity and other thermal properties, however, depend on internal degrees of freedoms. ▹ *degeneracy pressure*.

Incompressible The isothermal compressibility is defined by $1/\kappa_T(T, V) = -V\partial p(T, V)/\partial V$, in usual notation. A similar formula holds for the adiabatic compressibility. A fluid is (idealized) incompressible if its compressibility vanishes. The mass density in this case does not depend on pressure. In continuum physics, an incompressible fluid is characterized by a constant mass density. Mass conservation implies that the divergence of the velocity field vanishes, $\partial_i v_i = 0$. Water or hydraulic oil are nearly incompressible.

Inertial frame of reference A frame of reference consists of a good clock and a Cartesian coordinate system. It is an inertial system if bodies which are not acted upon by true forces move on straight lines with constant velocity. Since there is a maximal speed, namely that of light in vacuum, transformations from one to another inertial frame of reference are described by Einstein's special theory of relativity. In this book we consistently refer to the limit of small velocities which is described by ▷ *Galilei transformations*. Laws should be formulated in such a way that their meaning does not depend on the special inertial frame of reference. They should be equations between ▷ *tensor fields*.

Interaction picture ▷ *Time*.

Internal energy ▷ *Material points* carry kinetic, potential, and interior energy. There is a balance equation $\varrho\,\mathrm{D}_t\,u = -\partial_i J_i^{\mathrm{u}} + \pi^{\mathrm{u}}$ for the ▷ *specific* internal energy u. $\boldsymbol{J}^{\mathrm{u}}$ is the heat current density and π^{u} denotes the volumetric production rate for internal energy because of friction, Joule's heat, and other effects like radioactivity.

J

Johnson, John Bertrand: US-American electrical engineer, 1887–1970.

Johnson noise Electrons passing through an Ohmic resistor suffer friction by interacting with lattice vibrations. The other side of the same medal is that lattice vibrations produce spontaneous, random electric currents. Therefore, even in a completely passive electric circuit there is a thermal electromotive force producing noisy signals. This phenomenon was discovered by Johnson and explained by Nyquist. ▷ *Nyquist formula.*

Joule's heat Internal energy $E^{\mathrm{i}} = U$ may change with time because of five causes: inflow, compression, polarization, friction and the irreversible motion of charges counter to an electric field. The latter effect is called Joule's heat, it is the contribution $\boldsymbol{J}^{\mathrm{e}\,\prime\prime}\cdot\boldsymbol{E}$ to $\pi(U)$, the volumetric production rate of internal energy. $\boldsymbol{J}^{\mathrm{e}\,\prime\prime}$ is the irreversible part of the electric conduction current, the left hand side of ▷ *Ohm's law*.

K

Kelvin, Lord (William Thomson): British physicist, 1824–1907.

Kerr effect If an external quasi-static electric field $\boldsymbol{\mathcal{E}}$ is applied, the dielectric permittivity tensor will change. If a first order dependency is possible, it will dominate, ▷ *Pockels effect*. If however, the crystal under discussion has an inversion center, the second order term has to be taken into account. For an optically isotropic medium, the Kerr constant R is defined by $(\epsilon^{-1})_{ij} = (1/n^2)\delta_{ij} + R\mathcal{E}_i\mathcal{E}_j$ where n is the refractive index.

Khinchin, Alexandr: Russian mathematician, 1894–1959.

Khinchin's theorem ▷ *Wiener-Khinchin theorem.*

Kinetic coefficients Denote by X_s driving thermodynamic forces, normally gradients of equilibrium parameters such as temperature, flow velocity, chemical potentials, electric potential. They drive fluxes Φ_s which normally vanish in thermodynamic equilibrium. Heat currents, irreversible momentum flows T''_{ij} or diffusion currents are examples. Forces and fluxes are properly defined if the volumetric entropy production rate can be written as $\pi(S) = (1/T)\sum_r \Phi_r X_r$. For small departures from thermodynamic equilibrium one may write $\Phi_r = \sum_s K_{rs} X_s$. The matrix of kinetic coefficients K_{rs} is symmetric. Interchanging indexes r and s and inverting an external quasi-static magnetic field is a symmetry. ▹ *Onsager's relations*.

Kramers, Hans: Dutch physicist, 1894–1952.

Kramers-Kronig relation ▹ *Dispersion relation*.

Kronig, Ralph: German/US-American physicist, 1904–1995.

L

Lamb, Horace: British mathematician and physicist, 1849–1934. Mentioned in article *Reynold's Number*.

Lamé, Gabriel: French mathematician, 1795–1870.

Lamé constants ▹ *Hooke's law* for an isotropic elastic medium may be formulated as $T'_{ij} = 2\mu S_{ij} + \lambda\delta_{ij} S_{kk}$. S_{ij} is the strain tensor, S_{kk} its trace. The Lamé constants can be expressed in terms of ▹ *Young's modulus* and ▹ *Poisson's ratio* as $\lambda = E\nu/(1+\nu)(1-2\nu)$ and $\mu = E/2(1+\nu)$. Lamé's constants are normally used in wave equations, they are therefore adiabatic values.

Langevin equation A differential equation for a time dependent random variable. It usually contains a driving force which is described by its ▹ *spectral density*. See articles *Brownian Motion* and *Thermal noise* where the driving force is assumed to be ▹ *white noise*.

Langevin, Paul: French physicist, 1872–1946.

Laplace, Pierre-Simon: French mathematician and astronomer, 1749–1827.

Levi-Civita, Tullio: Italian mathematician, 1873–1941.

Lithium niobate A crystal of 3m symmetry with excellent acoustical and optical properties. It has a polar c-axis and therefore allows tensors of rank three which are symmetric in one pair of indexes. Consequently, the material shows a large ▹ *Pockels effect*, second harmonic generation (SHG, frequency doubling), direct and inverse piezoelectricity, acousto-optic effects, and so forth. When doped with erbium ions, lithium niobate becomes a laser material. When doped with iron ions, it shows a large photo-voltaic effect allowing for holographic information storage. Mentioned in articles *Bulk and Surface Acoustic Waves in Solids, Crystal Optics, Dielectric Planar Waveguides* and discussed in detail in *Pockels and Kerr Effect*.

Lorentz force An electromagnetic field $\boldsymbol{E}, \boldsymbol{B}$ exerts a force $\dot{\boldsymbol{p}} = q\{\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}\}$ on a particle with mass m, charge q and velocity $\boldsymbol{v}$. This force is responsible for the ▹ *Faraday effect* and the ▹ *Hall effect*.

Lorentz, Hendrik Antoon: Dutch physicist, 1853–1928.

Loschmidt, Johann Joseph: Austrian chemist and physicist, 1821–1895.

Loschmidt's number ▹ *Avogadro's number*.

Love, Augustus E.: English mathematician, 1863–1940.

Love wave An acoustic, horizontally polarized surface wave. Love waves travel faster than ▹ *Rayleigh waves*.

M

Material equation The set of ▹ *balance equations* is incomplete, it involves too many fields. Moreover, these balance equations are valid for properties of continuously distributed matter in general, irrespective of the particular substance involved. Material equations supplement the set of balance equations by relations between properties of ▹ *material points* which may contain parameters. Examples are ▹ *Ohm's law*, the condition for a ▹ *Newtonian fluid*, ▹ *Hooke's law*, but also expressions for ▹ *dielectric permittivities* or for the ▹ *degeneracy pressure* of a dense Fermi gas. Chapter 2 is an overview which is expanded in Chap. 4.

Material point The key notion of continuum physics. A material point is a region in space which is very small from an engineer's point of view. On the other hand, a material point contains such a huge number N of particles that the laws of equilibrium thermodynamic for $N \to \infty$ apply. These descriptions do not contradict in general. A rule of thumb says that relative fluctuations $\sqrt{N}/N$ should be negligible or at least less than 10^{-5}, the normal measuring accuracy. Read the corresponding section *Material Points* of Chap. 1.

Maxwell, James Clerk: Scottish physicist and mathematician, 1831–1879.

Maxwell's equations The equations which govern the electromagnetic field $\boldsymbol{E}, \boldsymbol{B}$, as set up by Maxwell, belong to the greatest achievements of science. Here the interaction of the electromagnetic field with continuously distributed matter is a main focus. In particular, optics as a discipline based on Maxwell's equations is dealt with in Chap. 3 and in various articles: *Crystal optics, Dielectric Planar Waveguides, Faraday Effect, Metamaterials, Optical Activity, Pockels and Kerr Effect and Surface Plasmon Polaritons*. Also read article *Ohm's Law and Hall Effect*. Maxwell's equations are presented and commented on in subsection *Digression on electromagnetism*.

Metamaterial Regular patterns of resonators with a distance much smaller than the wavelength of microwaves can be described by frequency dependent permittivity and permeability tensors. These may exhibit properties not found in natural materials, such as a negative refractive index. Advances in nano-technology and self-assembling may allow in the future to fabricate metamaterials also for optical applications such as ▷ *super lenses*. Read article *Metamaterials*.

Mixed state Systems containing many particles cannot properly be described by wave functions, or pure states. Instead, if $\phi_1, \phi_2, \dots$ is a complete set of mutually orthogonal (distinct) pure states, each of them occurs with a certain probability $w_1, w_2, \dots$ There is a self-adjoint linear operator W with eigenvectors ϕ_i and eigenvalues w_i. It describes a mixture of pure states, or a mixed state. Mixed states are characterized by $W \geq 0$, $\operatorname{tr} W = 1$ and by an ▷ *entropy* $S(W) = -k_{\mathrm{B}} \operatorname{tr} W \ln W$. ▷ *Boltzmann constant*. Read section *Statistical Thermodynamics*.

N

Navier, Claude-Louis: French physicist, 1785–1836.

Navier-Stokes equation The momentum balance equation for an ▷ *incompressible* ▷ *Newtonian fluid*, $\varrho\{\partial_t + \partial_j v_j\}v_i = -\partial_i p + \eta \Delta v_i$. p and v_i are the pressure and flow velocity fields, ϱ and η describe the constant mass density and the viscosity of the liquid. The flow behavior, whether creeping, laminar or turbulent, is characterized by geometrical details and ▷ *Reynold's number*. Read section *Fluid Media* and article *Reynold's Number*.

Newton, Isaak: English physicist and mathematician, 1642–1727.

Newtonian fluid $T_{ij} = -p\delta_{ij} + \eta\{\partial_i v_j + \partial_j v_i\}$ says that the medium is fluid and that frictional forces are proportional to velocity gradients. Water and hydraulic oil are well described as ▷ *incompressible* Newtonian fluids. There are differing reasons why a material does not behave as a Newtonian fluid. Either the relationship between frictional force and velocity gradient is retarded, as in glass, or non-linear, as in air.

Nyquist, Harry: US-American physicist and electrical engineer, 1889–1976. Mentioned in article *Thermal Noise*.

Nyquist formula An ohmic resistor generates white ▷ *Johnson noise*. The power $\mathrm{d}P$ in a frequency interval $\mathrm{d}f$ is $4Rk_{\mathrm{B}}T\,\mathrm{d}f$, so Nyquist's formula. R and T denote the resistor's resistance and temperature, respectively. The power is defined as $P(f) = \langle \tilde{V}(f)^2 \rangle$, where $\tilde{V}(f)$ is the Fourier transform of the noisy voltage across the resistor. Nyquist's formula allows to measure the Boltzmann constant k_{B}. Read article *Thermal Noise*.

O

Ohm's law Mobile electrons will move if they are dragged by an external field or if their concentration differs from location to location. Put otherwise, if the ▷ *electrochemical potential* ψ is not constant, its gradient causes electrons to move. Ohm's law states that the irreversible conduction current density is proportional to the negative gradient of the electrochemical potential, $J^{\mathrm{e}\,\prime\prime}_i = -\sigma_{ij}\,\partial_j \psi$. Without chemical effects Ohm's law reads $J_i^{\mathrm{e}\,\prime\prime} = \sigma_{ij} E_j$. This linear relationship between the electric current density and the gradient of the electrochemical potentials holds true for many orders of magnitude. The σ_{ij} are ▷ *conductivities*. They have to obey ▷ *Onsager's relations*.

Onsager, Lars: Norwegian/US-American physical chemist, 1903–1976.

Onsager relations Properly defined ▷ *susceptibilities*, ▷ *conductivities* or ▷ *kinetic coefficients* for cross-effects are described by symmetric matrices. Interchanging the indexes for cause and effect is a symmetry, provided a quasi-static external magnetic or induction field is inverted as well. Onsager's relations are a consequence of time reversal invariance. Read the corresponding section of Chap. 3.

Optical activity Crystals or suspensions of molecules with a screw structure show optical activity. The refractive indexes for left or right handed circularly polarized light beams differ by a small amount. A linearly polarized light beam passing through a probe of optically active material will leave it as a linearly polarized beam. But its polarization vector has been rotated by an angle which is proportional to the probe thickness. The phenomenon is similar to the ▷ *Faraday effect*. However, if the light beam is reflected and passes through the sample in reverse direction, the polarization rotation is undone. Read the corresponding article.

Optical isolator An ideal optical isolator is a device which transmits light in forward direction without loss and blocks it completely in backward direction. Only the ▷ *Faraday effect* allows for a non-reciprocal propagation of light. The standard device consists of a suitably arranged series of polarizer, Faraday rotator, polarizer, Faraday rotator and polarizer. The Faraday rotators rotate the plane of polarization by 45°. The polarizers let pass light at zero, 45° and 90°, respectively. Read the corresponding article for details. While micro-optical isolators are commercial products, their integrated optics counterparts are still the object of intensive research and development. The preferred material is suitably modified ▷ *yttrium iron garnet*.

P

Particles Although continuum physics is considered a discipline of classical physics, it is firmly embedded in quantum mechanics. The particles of a certain species, electrons say, can be counted, but not addressed individually. Particles of the same species are indistinguishable. N^a is the number of particles of species a, a ▷ *quantity*. Continuum physics therefore has to do with particle densities n^a, particle current densities $\boldsymbol{j}^a$ and volumetric production rates π^a only. Particles of a certain species are produced or annihilated in ▷ *chemical reactions*.

Pascal, Blaise: French mathematician, physicist and philosopher, 1623–1662.

Path A one-dimensional manifold in three-dimensional space. Also called a curve. Described by continuous and piecewise differentiable parameterizations $\boldsymbol{\xi}(s)$. At each point, $\boldsymbol{t}(s) = \mathrm{d}\boldsymbol{\xi}(s)/\mathrm{d}s$ spans a straight line, the tangent. A path has a starting and an end point. If they coincide, the path is closed. A path can be assigned a length which does not depend on the special parameterization for calculating it. Read more in Appendix A.

Pauli exclusion principle Particles of half integer spin, so called fermions, cannot occupy the same state more than once. Consequently, even at zero temperature, there is a ▹ *degeneracy pressure*. The Pauli exclusion principle also serves to explain the periodic table of elements.

Pauli, Wolfgang: Austrian/Swiss physicist, 1900–1958.

Peltier, Jean: French physicist, 1785–1845.

Peltier effect Consider a simple circuit of two wires of different material soldered together at P_1 and P_2. If an electric current is made to flow through this circuit, the temperatures at the soldering points will differ, the difference being proportional to the current. Read article *Thomson, Seebeck and Peltier effect*.

Perrin, Jean Baptiste: French physicist, 1870–1942.

Photonic crystals A photonic crystal is a material the optical permittivity of which varies in a regular pattern. Since the propagation of light is concerned, they are called photonic. They are called crystals because the permittivity modulations are regular, albeit the lattice constant is in the micrometer range, not nanometers. Photonic crystals can be arrays of regularly spaced identical rib waveguides (1D), arrays of boreholes (2D), or regularly staples of 2D photonic crystals. A photonic crystal in the narrower sense is a material with an optical band gap. A plane wave with wave vector $\boldsymbol{k}$ travels with an angular frequency $\omega = \omega(\boldsymbol{k})$. For a photonic crystal there is an interval of frequency values for which there is no wave vector. Waves of these forbidden frequencies cannot propagate in a photonic crystal giving rise to remarkable applications.

Pockels effect If a quasi-static electric field is applied, the dielectric permittivity changes, in lowest order, by an amount which is proportional to $\boldsymbol{\mathcal{E}}$. This electrooptic Pockels effect is described by $(\epsilon^{-1})_{ij} = (\epsilon^{-1})^0_{ij} + r_{ijk}\mathcal{E}_k + \dots$ A tensor r_{ijk} of rank three which is symmetric in the first index pair is possible only if the crystal has no inversion center. ▹ *Lithium niobate* is an example. In article *Pockels and Kerr effect* we study the corresponding crystal symmetry group 3m in detail. The dots in the above expression indicate an addition which is quadratic in $\boldsymbol{\mathcal{E}}$ describing the ▹ *Kerr effect*.

Pockels, Friedrich: German physicist, 1865–1913.

Poiseuille, Jean: French physician and physiologist, 1797–1869. ▹ *Hagen-Poiseuille law*.

Poisson, Siméon Denis: French mathematician and physicist, 1781–1840.

Poisson's ratio A column of height h and square cross section $A = \ell^2$ is fixed at the bottom and pressed upon at the top with a force $F = pA$. The relative height change $\delta h/h$ is p/E, which defines ▹ *Young's module* E. The relative lateral dimension change $\delta\ell/\ell$ is written as $\nu p/E$. This defines Poisson's ratio ν. By applying pressure, the column's volume should not increase, which amounts to $0 \le \nu \le 1/2$. $\nu = 1/2$ says that the volume does not change; rubber is an example. Normal metals and other common construction materials, such as steel, are characterized by $\nu \approx 0.3$. Read section *Solid Media* of Chap. 2.

Pressure A ▹ *fluid*, gaseous or liquid, cannot exert shear stress if the medium is at rest. Its stress tensor, precisely its reversible contribution, is proportional to the unit tensor multiplied by $-p$, where p denotes the pressure field. If there is a shear force, it results from friction. Thermodynamic stability demands that pressure p is never negative. Pressure is a force per unit area or energy density, its SI unit is Pa (Pascal). ▹ *incompressible*, ▹ *ideal gas*, ▹ *degeneracy pressure*, ▹ *free energy*.

Q

Quality As contrasted with ▹ *quantity*, this word describes properties of material points for which adding makes no sense. Examples are temperature, pressure, chemical potential, electric potential and so forth. In thermodynamic terminology, variables describe a quality if they are intensive. They remain the same if systems in equilibrium are joined. A ▹ *specific* quantity is a quality.

Quantity Within the framework of continuum physics, quantity refers to an observable property of a system which can be added and transported. ▹ *Particles* of a certain species, mass, charge, momentum, kinetic, potential and internal energy as well as entropy are examples. For each quantity Y there is a ▹ *density* $\varrho(Y) = \varrho(Y; t, \boldsymbol{x})$, a ▹ *current density* $\boldsymbol{j}(Y) = \boldsymbol{j}(Y; t, \boldsymbol{x})$ and a ▹ *volumetric production rate* $\pi(Y) = \pi(Y; t, \boldsymbol{x})$ which obey a ▹ *balance equation*. In thermodynamic terminology, quantities are extensive. They add if systems are joined.

R

Rayleigh, Lord (John William Strutt): British physicist, 1842–1919.

Rayleigh wave A surface acoustic wave with vanishing transversal component of the displacement field. It travels slower than a bulk acoustic wave in the same medium. Its energy remains concentrated below the surface, i.e., it decays proportional to the inverse distance between source and receiver. Read article *Bulk and Surface Acoustic Waves*.

Reaction-diffusion Interesting and surprising solutions show up if several kinds of particles locally undergo chemical reactions and propagate by diffusion. Here the ▹ *Gray-Scott model* is discussed in some detail. Read the corresponding article.

Reynold, Osborne: British physicist, 1842–1912.

Reynold's number With ϱ the mass density and η the viscosity of an incompressible fluid, $\texttt{Re} = \varrho v \ell/\eta$ is a dimensionless number. v denotes a typical velocity and

ℓ a typical length of a problem. Problems with the same Reynold number $\mathtt{Re}$ have similar solutions. Laminar flow is characterized by a small Reynold number, large values indicate turbulence.

S

Scalar field A field S with only one component is a scalar field if $S(t,\boldsymbol{x}) = S'(t',\boldsymbol{x}')$ holds true. Primed objects refer to the new inertial system, unprimed to the old. Time and space coordinates are related by the ▹ *Galilei transformation* $t = t' + \tau, \boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'$. A scalar transforms as a constant scalar field. Read more in Appendix A.

Schottky, Walter: German physicist, 1886–1976. Mentioned in article *Thermal Noise of a Resistor.*

Schrödinger, Erwin: Austrian physicist, 1887–1961.

Schrödinger picture ▹ *Time.*

Second main law The so-called second main law of thermodynamics states that the volumetric production rate $\pi(S)$ of entropy S is never negative. There are many sloppier formulations of it. "There is no *perpetuum mobile of the second kind*", a machine which will not cease to move without making use of temperature differences. Or, "disorder ever increases". We prove, in section *Fluctuations and Dissipation* of Chap. 3, that a system interacting with an electromagnetic field always absorbs field energy. This is rather close to a proof of the second main law since the reasoning can easily be generalized to more general perturbations of the equilibrium.

Seebeck, Thomas Johann: Baltic-German physicist, 1770–1831.

Seebeck effect Consider a simple circuit of two wires of different material soldered together at P_1 and P_2. If the soldering points are kept at different temperatures T_1 and T_2, respectively, an electric current is invoked which is proportional to the temperature difference. Read article *Thomson, Seebeck and Peltier effect.*

Sellmeier, Wolfgang: German physicist.

Sellmeier formula The refractive part of the permittivity is an integral of the absorptive part, ▹ *Kramers-Kronig relation*. Contributions come from absorption bands which are represented by a central frequency and a weight. Sellmeier's formula is a representation of the permittivity by pole contributions. Read article *Crystal Optics.*

Shear modulus $G = E/2(1+\nu)$ appears in torsion problems. E is ▹ *Young's modulus* and ν denotes ▹ *Poisson's ratio*. Formally, the shear modulus coincides with the ▹ *Lamé constant* μ. However, the former refers to isothermal, the latter to adiabatic deformations.

Specific A certain physical quantity Y per unit mass. Denoted generically by $\sigma(Y)$. With $\varrho = \varrho(M)$ as mass density and $\varrho(Y)$ as density of Y, we may write $\varrho(Y) = \varrho\,\sigma(Y)$. In this book we reserve the word *specific* consequently as referring to unit mass. Exceptions are the specific rotations of the polarization vector which are meant per unit optical path length. ▹ *Faraday effect* and ▹ *optical activity*.

Spectral density ▹ *Wiener-Khinchin theorem*.

Stefan, Jožef: Slovenian/Austrian physicist, 1835–1893.

Stoichiometric coefficients In a chemical reaction like $2H_2+O_2 \rightarrow 2H_2O$, two H_2 and one O_2 molecules vanish while two H_2O molecules appear. This reaction is characterized by the stoichiometric coefficients $\nu^1 = -2$, $\nu^2 = -1$ and $\nu^3 = 2$. The superscripts $a = 1, 2, 3$ stand for H_2, O_2 and H_2O molecules, respectively. Negative stoichiometric coefficients mean disappearance, positive values indicate creation. The stoichiometric coefficients have no common divisor. Stoichiometric coefficients ν^{ra} refer to a reaction of type r. ▹ *Chemical reaction*.

Stokes, George: British physicist and mathematician, 1819–1903. ▹ *Navier-Stokes equation*. Read article *Stokes' Law*.

Strain An elastic solid, if relaxed, is described by its ▹ *material points* at locations $\boldsymbol{x}$ at time t. If it s acted upon, the same material points become located at $\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{u}(t, \boldsymbol{x})$. However, a translation or rigid rotation does not really affect the material. We therefore calculate distances between neighbored points $\boldsymbol{x}'$ and $\boldsymbol{x}' + \mathrm{d}\boldsymbol{x}'$. In linear approximation it is given by $|\mathrm{d}\boldsymbol{x}'|^2 = |\mathrm{d}\boldsymbol{x}|^2 + S_{ij}\,\mathrm{d}x_i\,\mathrm{d}x_j$. The symmetric tensor field $S_{ij} = S_{ij}(t, \boldsymbol{x})$ characterizes the strain. Note that S_{ij} vanishes if the medium is translated or rigidly rotated.

Stress Momentum P_j may be transported by convection and conduction. The conduction current density $J_i(P_j) = -T_{ij}$ defines the stress tensor T_{ij}. The force exerted by the medium on the front size of a surface element $\mathrm{d}A_i$ is $\mathrm{d}F_j = \mathrm{d}A_i\,T_{ij}$. The stress tensor appears in the momentum balance equation $\varrho\,\mathrm{D}_t\,v_i = \partial_j T_{ij} + f_i$, where ϱ is the mass density, v_i the velocity field and $\pi(P_i) = f_i$ the external force per unit volume. The stress tensor may be split into an elastic, or reversible part T'_{ij} and an inelastic, or irreversible contribution T''_{ij}. Angular momentum conservation demands that both parts are symmetric.

Strutt, John William (Lord Raleigh): British physicist, 1842–1919.

Super lens An optical imaging device the resolution of which is not limited by diffraction. It may be realized with future ▹ *metamaterials* of negative index of refraction. A conventional lens (e.g., of an optical microscope) provides only the information surviving in the far field while super lenses analyze the near field. Read article *Metamaterials*.

Surface A two-dimension manifold in three-dimensional space. Sometimes also called an area. Described by piecewise differentiable parameterizations $\boldsymbol{\xi}(s_1, s_2)$. At each point of the surface, there are two non-vanishing tangential vectors $\boldsymbol{t}_1 = \partial\boldsymbol{\xi}/\partial s_1$ and $\boldsymbol{t}_2 = \partial\boldsymbol{\xi}/\partial s_2$ which span a plane. $\boldsymbol{n} = \boldsymbol{t}_1 \times \boldsymbol{t}_2$ defines the normal vector.

Its direction does not depend on the particular parameterization. A surface $\mathcal{A}$ has a boundary $\partial\mathcal{A}$, a closed path. The surface is closed if its boundary curve vanishes. Read more in Appendix A.

Surface plasmon polaritons The surface of a high ▹ *conductivity* metal, which is covered by air or another dielectric medium, may carry a ▹ *guided optical wave* of ▹ *transverse magnetic* polarization. It is localized within a few tens of nanometers close to the surface. The electromagnetic wave is in resonance with a polarization wave of the conduction band plasma. One speaks of polaritons because the plasma oscillations behave as quasi-particles. For low enough photon energies, the ▹ *Drude model* describes the ▹ *dielectric susceptibility* well, at least for noble metals such as gold. Read the corresponding article.

Susceptibility ▹ *Dielectric susceptibility* for a definition in the narrow sense. Generally, a system with a time-dependent Hamiltonian $H_t = H - \sum_s \lambda_s(t) V_s$ responds by time-dependent expectations values $\langle V_r \rangle_t = V_r(t)$. Their Fourier transforms depend linearly on the Fourier transforms of the driving parameters, $\tilde{V}_r(\omega) = \sum_s \chi_{rs}(\omega)\tilde{\lambda}_s(\omega)$. The proportionality factors χ_{rs} are generalizes susceptibilities. They obey ▹ *dispersion relations* and ▹ *Onsager relations*. The susceptibilities depend not only on angular frequency, but on all parameters which affect the thermodynamic equilibrium, such as temperature, stress, quasi-static external electric and magnetic fields, and so forth.

T

Temperature The equilibrium, or ▹ *Gibbs states* of a system in contact with its environment is characterizes by maximal ▹ *entropy*. The corresponding optimization must take auxiliary conditions into account: the searched for state has to be normalized, $\operatorname{tr} G = 1$, and its internal energy $U = \operatorname{tr} GH$ is prescribed. One Lagrange parameter is the free energy, the other one the temperature of the system. It follows that temperature is well defined only for equilibrium states, for example, of a ▹ *material point*. Read section *Statistical Thermodynamics*.

Tensor field Functions $T_{ij\dots} = T_{ij\dots}(t, \boldsymbol{x})$ with N indexes transform are tensor fields of rank N. Upon a ▹ *Galilei transformation* $t = t' + \tau$ and $\boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'$ the tensor transforms as $T_{ij\dots}(t, \boldsymbol{x}) = R_{im} R_{jn} \cdots T'_{mn\dots}(t', \boldsymbol{x}')$. Tensors of rank zero are scalars. Tensors of rank one are called vectors. Tensors of rank two are proper tensors. The Kronecker symbol δ_{ij} is a constant tensor of rank 2. Equations between tensor fields of the same rank prevail in this book, they guarantee that laws formulated in this way are valid irrespective of a special inertial frame of reference.

Tesla, Nikola: Serbian mechanical and electrical engineer, 1856–1943.

Thermal conductivity ▹ *Fourier's law*.

Thermal diffusivity ▹ *Heat equation*.

Thomson effect The density of internal energy may change because of a net heat inflow, ▹ *Joules heat*, and a third term $\mu \boldsymbol{J}^{\mathrm{e}} \cdot \nabla T$. This contribution, which describes the Thomson effect, is proportional to an electric current and a heat gradient. It changes sign if the electric current is reversed. μ is the Thomson coefficient of the electric conductor. Read article *Thomson, Seebeck and Peltier effect*.

Thomson, William (Lord Kelvin): British physicist, 1824–1907.

Time Time in physics is usually the time span t between preparing a state W and measuring an observable property M. Waiting is described by a family of unitary operators U_t. In the Schrödinger picture, preparing W and waiting defines a new state $W_t = U_t W U_{-t}$. In the Heisenberg picture, waiting and measuring M defines a new observable $M_t = U_{-t} M U_t$. Both views are equivalent because of $\operatorname{tr} W_t M = \operatorname{tr} W M_t$. The interaction picture is useful if the Hamiltonian splits into a manageable part H and a perturbation V. The transformation from Schrödinger's to the interaction picture is performed with H only instead of $H + V$. Read section *Perturbations* of Chap. 3.

Time reversal The transformation $t \to -t$ refers to relations between physical objects explicitly or implicitly depending on ▹ *time t*. Because of $\boldsymbol{x} \to \boldsymbol{x}$ and $\dot{\boldsymbol{x}} \to -\dot{\boldsymbol{x}}$ the transformation is also called reversal of motion. ▹ *Maxwell's equations* as well as the ▹ *Lorentz force* are compatible with time reversal. The ▹ *Second Law of Thermodynamics*, namely $\pi(S) \geq 0$, is not because the initial condition $W_t \to G$ for $t \to -\infty$ has been implemented which breaks time reversal invariance. Read section *Onsager Relations* of Chap. 3.

Transverse electric, magnetic A planar dielectric waveguide is characterized by $\mu = 1$ and $\epsilon = \epsilon(x)$. Guided modes travel in z direction. Thus the $x - z$ plane is singled out. If the electric field is perpendicular to this plane, we speak of a TE mode, transverse electric. Likewise, if the magnetic field is perpendicular, the guided mode is called TM. This terminology also applies to linear waveguides if they are much broader than high. For linear waveguides of circular cross section, like glass fibers, a distinction between TE and TM makes no sense.

Turing, Alan: British mathematician and computer scientist, 1912–1954. Mentioned in article *Reactions and Diffusion*.

U

Universal gas constant Any gas, at low enough density, behaves ideally. Pressure p, volume V, absolute temperature T and the number N of particles are related by $pV = NRT$. With $n = N/N_\mathrm{A}$ as the number of moles, this may be rewritten as $pV = nRT$. $R = 8.314\ \mathrm{J\,K^{-1}\,mol^{-1}}$ is the universal gas constant, N_A denotes ▹ *Avogadro's number*.

V

Vector field A field V_i with three components is a vector field if $V_i(t, \boldsymbol{x}) = R_{ij} V'_j(t', \boldsymbol{x}')$ holds true. Primed objects refer to the new inertial system, unprimed to the old. Time and space coordinates are related by the ▹ *Galilei transformation* $t = t' + \tau, \boldsymbol{x} = \boldsymbol{a} + R\boldsymbol{x}' + \boldsymbol{u}t'$. A vector transforms as a constant vector field.

Verdet, Émile: French physicist, 1824–1866. Mentioned in article *Faraday Effect*.

Viscosity Adjacent layers of a fluid exert shear forces if the flow with different velocities. An incompressible ▹ *Newtonian fluid* is characterized by $T''_{ij} = \eta^{\mathrm{s}}(\partial_i v_j + \partial_j v_i)$, the coefficient η^{s} being the shear viscosity. For a compressible fluid, a bulk viscosity coefficient η^{b} must also be taken into account. Read section *Fluid Media*. Viscosity describes internal friction, an irreversible effect.

Volta, Allesandro: Italian physicist and chemist, 1775–1827.

Volume A three-dimension manifold in three-dimensional space. Sometimes also called a region. Described by piecewise differentiable parameterizations $\boldsymbol{\xi}(s_1, s_2, s_3)$. At each point of the volume, there are three linear independent tangential vectors $\boldsymbol{t}_k = \partial\boldsymbol{\xi}/\partial s_k$. The boundary $\partial\mathcal{V}$ of a volume $\mathcal{V}$ is a closed surface. The content $V = \mathrm{vol}(\mathcal{V})$ of a volume is also called its volume. Read more in Appendix A.

Volumetric production rate The quantity Y in a certain volume changes because of outflow and production. The former is described by the current $I(Y)$ across the surface, the latter by the production rate. This rate may be written as an volume integral of a volumetric production rate $\pi(Y) = \pi(Y; t, \boldsymbol{x})$ which is a scalar field. The volumetric production rate appears in the generic ▹ *balance equation* $\partial_t \varrho(Y) + \partial_i j_i(Y) = \pi(Y)$. $\pi(M)$ and $\pi(Q)$ (mass and electric charge) always vanish. Particles of a certain species may be produced in chemical reactions. The volumetric production rate for momentum P_i is nothing else than the external force per unit volume, $\pi(P_i) = f_i$. Kinetic, potential and internal energy and entropy may be produced as well.

W

White dwarf A normal star, like our sun, will finally become instable because its hydrogen fuel has been fused into helium ash. The hydrostatic equilibrium between gravitational pull and thermal pressure can no longer be maintained, and the star suffers a series of relatively rapid transitions. In the end, the star is either a white dwarf, a neutron star, or a black hole. A plasma of positively charged carbon and oxygen nuclei and negatively charged electrons exerts a ▹ *degeneracy pressure* which is able to stabilize the star, even for low or vanishing temperature. However, the star's mass must not exceed ▹ *Chandrasekhar's limit*. White dwarfs are dwarfs, since the sun will be as large as the earth, and appear white because the remnant energy is to be radiated off a comparatively small surface. Read article *White Dwarfs*.

White noise If a fluctuation now is not correlated with the fluctuation a short time later, one speaks of white noise. Consider the process $t \to M_t$ where the M_t are time-dependent random variables (in the language of classical physics) or observables (in the terminology of quantum physics). $\delta M_t = M_t - \langle M_t \rangle$ is a fluctuation, the deviation from the mean value. $K(\tau) = \langle \delta M_{t+\tau} \delta M_t \rangle$ or a similar expression in quantum theory denotes the time-correlation function which, for a stationary state, depends on the time span τ only. The ▷ *Wiener-Khinchin theorem* guarantees that the correlation function is the Fourier transform of the process' spectral density, a positive function. If the spectral density does not depend on frequency, or if the correlation function may be approximated by a δ-function, the fluctuation behaves as white noise. Mentioned in articles *Brownian Motion* and *Thermal Noise of a Resistor*.

Wiener, Norbert: 1894–1964, US-American mathematician.

Wiener-Khinchin theorem Consider a stationary state of a system and a process M_t. M is an observable depending on time t. Its fluctuation is $\delta M_t = M_t - \langle M \rangle$. Note that $\langle M_t \rangle = \langle M \rangle$ does not depend on time. The time correlation function $K(\tau) = \langle \delta M_{t+\tau} \delta M_t \rangle$ likewise does not depend on time t. The Wiener-Khinchin theorem states that the Fourier transform $S = S(\omega)$ of the time correlation function $K = K(\tau)$ is nowhere negative. $S = S(\omega)$ is the spectral density of the process under consideration. Read section *Fluctuation and Dissipation* and articles *Brownian Motion and Thermal Noise of a Resistor*.

Y

Yttrium iron garnet An artificially grown crystal (YIG) with interesting magnetooptic properties. $Y_3Fe_2(FeO_4)_3$ is ferrimagnetic. There are two oppositely magnetized sub-lattices. The crystal is transparent in the infrared region used for glass fiber communication applications. By doping it with rare earth ions, it acquires interesting magnetooptic properties, such as a large specific Faraday rotation. YIG is the preferred material for an integrated ▷ *optical isolator*. Read article *Faraday Effect*.

Young, Thomas: British physicist and physiologist, 1773–1829. Also known for deciphering the Rosette stone.

Young's modulus A column of height h and cross section A is fixed at the bottom and pressed upon at the top with a force $F = pA$. The relative height change $\delta h/h$ is p/E, which defines the elasticity, or Young's modulus E. ▷ *Poisson's ratio*. Read section *Solid Media* of Chap. 2 and article *Elasticity Modules*.

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