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General Theory and Applications to Schrödinger and Dirac Equations with Singular Potentials

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Preface

Quantization of physical systems includes a correct definition of physical observables (such as the Hamiltonian and the momentum) as self-adjoint operators in an appropriate Hilbert space and their proper spectral analysis. A solution of this problem is not a straightforward and unambiguous procedure for nontrivial quantum systems (systems on nontrivial manifolds, in particular on manifolds with boundaries or with singular interactions). Quantum-mechanical models with singular potentials, both relativistic and nonrelativistic, and/or with boundaries, play an important role in physics. A consistent treatment of nontrivial quantum systems is beyond the scope of the mathematical apparatus in standard textbooks on quantum mechanics (QM). But a "naïve" treatment based on finite-dimensional linear algebra or even on the theory of bounded operators can result in paradoxes and incorrect results. Some paradoxes due to a "naïve" treatment demonstrate that even simple physical models can be nontrivial from the mathematical standpoint. It is well known that a rigorous pure-mathematical approach to constructing physical observables in nontrivial quantum systems leads to a result that is not unique. Additional physical arguments must eventually be used to choose a proper quantization for a given physical system. An application of the technique of self-adjoint extensions of symmetric operators makes the inherent nonuniqueness obvious and facilitates a physically proper choice.

In this book, we focus on the problem of a correct definition of quantum-mechanical observables, which is an important part of operator quantization. We show how this problem can be solved for comparatively simple but nontrivial quantum-mechanical systems. The solution of the above problem requires invoking some nontrivial notions of functional analysis concerning the theory of linear operators in Hilbert spaces, in particular, the notions of unbounded self-adjoint operators and their spectral analysis and of self-adjoint extensions of symmetric operators. The general theory is then illustrated on a number of physical examples. In particular, it is shown how the problem of a correct definition of observables is solved for a free one-dimensional particle on the whole axis, on a semiaxis, and on a finite interval. In addition, various nontrivial quantum systems are treated in accordance with the general mathematical theory of self-adjoint extensions and a rigorous spectral theory. These are the one-dimensional particles in the Calogero potential and in the potentials localized at the origin, in particular, deltalike potentials. Additionally, a rigorous treatment of the Schrödinger operators with all the so-called exactly solvable potentials is given, and the relativistic problem for an electron in the Coulomb field of arbitrary (including supercritical) charge is considered in detail. A similar analysis is carried out for nonrelativistic and relativistic electrons in the Aharonov–Bohm field and in the so-called magnetic-solenoid field.

The book is addressed to readers who are interested in deepening their understanding of mathematical problems in QM beyond the scope of standard textbooks.

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Contents

Chapter 1
Introduction

1.1 General Remarks

Among different approaches to constructing a quantum description of physical systems and its proper interpretation, operator quantization is the oldest and most-used one. The main first-stage problem of operator quantization is the problem of a correct definition of observables as self-adjoint operators (s.a. operators in what follows) in an appropriate Hilbert space. The self-adjointness of observables is of crucial importance for quantum theory (QT). An s.a. operator possesses a real-valued spectrum and a complete orthogonal set of (generalized) eigenvectors in the corresponding Hilbert space. These properties of any observable provide a basis for the probabilistic interpretation of QT (in particular, quantum mechanics (QM), which is the principal object of our consideration). The problem of a correct definition of quantum observables is generally nontrivial in the case of physical systems with boundaries and/or with singular interactions (including QFT models). In what follows, for the sake of brevity, we call such systems *nontrivial physical systems* (or simply nontrivial systems). The interest in this problem revives periodically in connection with studies of specific nontrivial systems such as a particle on a finite interval or on a semiaxis, a particle in singular potential fields, in particular in the Aharonov–Bohm or in δ-like potential fields, and so on. The reason is that the solution of the problem, and therefore a consistent QM treatment of nontrivial systems, requires a considerable amount of preliminary information from different advanced chapters of functional analysis. However, the content of such chapters usually goes beyond the scope of the mathematical apparatus presented in standard textbooks on QM for physicists,[1] e.g., [32, 39, 44, 48, 64, 104, 109, 112, 136, 138] and even in recently published textbooks [23, 37, 63, 98].

[1]The exceptions such as [27, 57, 83, 84, 128, 144, 147, 153] are mainly intended for mathematically minded physicists and mathematicians.

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One of the aims of this book is of a pedagogical nature, namely, to convince the reader–physicist that he or she must be very careful when reading standard textbooks on QM for physicists, and particularly careful when applying the notions and prescriptions from such textbooks to nontrivial systems as regards the mathematical apparatus of QM.

The mathematical apparatus of QM is functional analysis, more specifically, the theory of linear operators in Hilbert spaces. It is a quite extensive and "subtle" science, so it takes considerable time to master it. For this reason, standard textbooks on QM for physicists present a rather simplified version of the relevant parts of functional analysis in the form of brief "rules" such that many mathematical subtleties are necessarily left aside. The simplified rules are usually based on systematic references to our experience in finite-dimensional linear algebra, which often proves to be misleading. We recall these rules below. They can be sufficient as long as we examine comparatively simple QM systems. But if we follow these rules literally in our treatment of even the simplest nontrivial systems (in what follows, we call this approach the *naïve treatment*), we encounter some paradoxes that may lead us to incorrect conclusions. In this chapter, we present a number of such paradoxes, and a resolution of them is given in subsequent chapters.

As stated above, QM generally and a consistent QM treatment of nontrivial systems particularly require the language of the theory of linear operators in Hilbert spaces and realizing subtleties associated with unbounded operators, in particular, with such basic notions as a closed operator, an adjoint operator, a symmetric operator, and an s.a. operator,[2] the spectrum of an s.a. operator and its spectral decomposition, the so-called inversion formulas for s.a. differential operators, and so on. Another aim of this book is to remind the reader–physicist of (or provide an introduction to) these notions and some related subjects.

A crucial subtlety is that an unbounded s.a. operator cannot be defined in the whole Hilbert space, i.e., on an arbitrary QM state, which is usually assumed in a preliminary "idealized" scheme of operator quantization. But there is no operator without its domain of definition: an operator is not only a rule of acting, but also a domain in a Hilbert space to which this rule is applicable. In the case of unbounded operators, the same rule for different domains generates different operators with sometimes completely different properties. Provided a rule of acting is given, it is an appropriate choice of a domain for a QM observable that makes it an s.a. operator. The main problems are related to this point. The formal rules of operator canonical quantization (see below) are of a preliminary nature and generally provide only "candidates" for unbounded QM observables, so to speak, for example in the form of the so-called s.a. differential operations,[3] because their domains are not prescribed by the canonical quantization rules. Appropriate domains even are not clear at the first stage of quantization, especially in the case of nontrivial physical systems,

[2]For unbounded operators, there is a crucial difference between the notions of symmetric (Hermitian) and s.a. operators; for bounded operators, these notions actually coincide.

[3]S.a. according to Lagrange in mathematical terminology; see Chap. 4.

although it is prescribed that observables must be s.a. operators. It should be noted that the choice of domains providing the self-adjointness of all observables involved, especially the primarily important observables such as the position, momentum, Hamiltonian, and symmetry generators, is a necessary part of quantization resulting in a specification of a QM description of a physical system in question. This is actually a physical problem. Mathematics can only help a physicist in making a choice by indicating various possibilities.

It is expected that for physical systems whose classical description includes infinite (but finite-dimensional) flat phase spaces such as $\mathbb{R}^{2n}$ and nonsingular interactions, a quantization is practically unique: the most important physical observables are defined as s.a. operators on some "natural" domains; in particular, classical symmetries can survive under quantization. The majority of textbooks for physicists begin their exposition of QM with a treatment of such physical systems. Of course, nontrivial physical systems are also examined thereafter. Nevertheless, the common belief is that no actual singularities exist in nature. They are the products of our idealization of reality, i.e., are of a model nature, which is related, for example, to our ignorance of the details of interaction at small distances. We formally extend an interaction law known for finite distances between finite objects to infinitely small distances between pointlike objects. We treat boundaries as a result of infinite potential walls that are actually always finite.[4] The consequence is that singular problems in QM are commonly solved via some regularization considered to be natural and then via a subsequent limiting process of removing the regularization. In some cases, this procedure requires the so-called infinite renormalization (of coupling constants, for example). But in some cases, no reasonable limit is known. (It should be pointed out that here, we mean conventional QM rather than quantum field theory.) It may also happen that different regularizations yield different physical results. It is precisely the case in which mathematics can help a physicist with the theory of s.a. extensions of symmetric operators. This was first recognized by Berezin and Faddeev [26] in connection with the three-dimensional δ-potential problem.

The practice of quantizing nontrivial systems shows that preliminary candidates for observables can be quite easily assigned symmetric operators defined on such domains that "avoid" problems: they do not "touch" boundaries and "escape" any singularities of interaction; this is a peculiar kind of "mathematical regularization." But such symmetric operators are commonly non-s.a. The main question then is whether these preliminary observables can be assigned s.a. operators by some extensions of the initial symmetric operators that convert the candidates to real observables. The answer is simple, positive, and unique if a symmetric operator under consideration is bounded. However, if it is unbounded, the problem is generally nontrivial.

[4] Of course, a flat infinite space is also an idealization, as is any infinity.

The theory of s.a. extensions of unbounded symmetric operators provides the main tool for solving this problem. It turns out that these extensions are generally nonunique, if they are possible at all. From the physical standpoint, this implies that when quantizing a nontrivial physical system, we are generally presented with different possibilities for its quantum description. The general theory describes all the possibilities that mathematics can offer to a physicist. Of course, a physical interpretation of available s.a. extensions is a purely physical problem. Any extension is a certain prescription for the behavior of a physical system under consideration near its boundaries and singularities. We also believe that each extension can be understood through an appropriate regularization and a subsequent limiting process, although this is generally a complicated problem in itself. But in any case, the right of a final choice belongs to the physicist.

The book is organized as follows. In the introduction, we demonstrate that an idealized scheme of operator canonical quantization applied to nontrivial systems can lead to a number of paradoxes. Chapters 2 and 5 (purely mathematical chapters in a sense) contain all the information about Hilbert spaces, linear operators in such spaces, and a strict formulation of the spectral problem for s.a. operators that physicists need and that is used in the book. This standard material is followed by the general theory of s.a. extensions of symmetric operators presented in Chap. 3. The traditional exposition (due to von Neumann) is accompanied by a nontraditional approach that is based on the notion of asymmetry forms generated by adjoint operators, see our works [156, 157]. The basic statements concerning the possibility and specification of s.a. extensions both in terms of isometries between the deficient subspaces and in terms of the sesquilinear asymmetry form are collected in the main theorem. It is followed by a comment on a direct application of the main theorem to physical problems of quantization. We outline a possible general scheme of constructing QM observables as s.a. operators starting from initial formal expressions supplied by canonical quantization rules. The subsequent Chap. 4 is devoted to the exposition of specific features and appropriate modifications of the general theory as applied to ordinary (one-dimensional) differential operators in Hilbert spaces $L^2(a,b)$ [158]. For symmetric differential operators, the isometries between deficient subspaces specifying s.a. extensions can be converted to s.a. boundary conditions, explicit or implicit, based on the fact that asymmetry forms are expressed in terms of the (asymptotic) boundary values of functions and their derivatives. We describe various ways of specifying s.a. operators by s.a. boundary conditions depending on the regularity or singularity of the ends of the interval under consideration. In particular, we propose a new method for specifying s.a. ordinary differential operators by s.a. boundary conditions based on evaluation of the quadratic asymmetry form in terms of asymptotic boundary coefficients. A comparative advantage of the method is that it makes it possible to avoid the evaluation of deficient subspaces and deficiency indices. Its effectiveness is illustrated in Chaps. 6–10 with examples of constructing QM observables for a number of nontrivial systems. In Chaps. 6–8, we consider various one-dimensional systems: a free particle on a semiaxis and on a segment of the real axis (Chap. 6), a particle in different potential fields including the Calogero potential, deltalike potentials, and so-called exactly solvable potentials (Chaps. 7 and 8). In Chaps. 9 and 10, we study certain one-particle three-dimensional problems. In Chap. 9, we consider a Dirac particle moving in the Coulomb field of a point charge Ze. We interpret the Dirac equation with the Coulomb field as the Schrödinger equation; the corresponding quantum Hamiltonian is called the Dirac Hamiltonian. We define the Dirac Hamiltonian with the Coulomb field as an s.a. operator for any real Z and solve the corresponding spectral problem. In Chap. 10, we similarly examine the Dirac Hamiltonian with the Aharonov–Bohm field and with the so-called magnetic-solenoid field.

1.2 Idealized Scheme of Operator Canonical Quantization

For a physicist, quantization means constructing a QT for a given physical system on the basis of an initial classical theory and in accordance with the correspondence principle. The correspondence principle requires that the QT must reproduce the predictions of the initial classical theory in the classical limit (large masses, macroscopic scales, smooth potentials, and so on), which is formally the limit $\hbar \to 0$, where $\hbar$ is the Planck constant.[5] The quantization problem usually does not have a unique solution. The only criterion for whether a constructed QT is proper remains the coincidence of its predictions with experiment. The development of QT began with the quantization of the simplest systems such as a free particle, a harmonic oscillator, and a nonrelativistic particle in some potential fields. In fact, the experience in the quantization of such systems was used to formulate a consistent general scheme of operator quantization for an arbitrary system with canonical Hamiltonian equations of motion for phase-space variables. It is this scheme that was called canonical quantization. In what follows, we outline the canonical quantization rules as they are usually expounded in standard textbooks on QM for physicists. This is a "first approximation" to a proper quantization, so to speak, the naïve treatment, as was already mentioned before, or *the idealized scheme of operator canonical quantization*. In short, this scheme is as follows.

(a) It is assumed that there exists a canonical Hamiltonian formulation of the classical mechanics of a physical system under consideration. This means that a state of the system at any instant of time is specified by a point of some even-dimensional phase space; the points of this space are labeled by canonical generalized coordinates x^a and momenta p_a, $a = 1, \ldots, n$, where n is the number of degrees of freedom. The time evolution of a state of the system in the course of time t is described by the Hamiltonian (canonical) equations of motion for the canonical coordinates $x^a(t)$ and $p_a(t)$:

$$\dot{x}^a = \{x^a, H\}, \; \dot{p}_a = \{p_a, H\},$$

[5]For a mathematician, quantization is a quantum deformation of classical structures; the deformation parameter is the Planck constant $\hbar$.

where $H = H(x, p)$ is the Hamiltonian of the system and $\{\,,\,\}$ is the canonical Poisson bracket. The canonical Poisson bracket of two arbitrary functions f and g on the phase space is defined by

$$\{f, g\} = \sum_a \left(\frac{\partial f}{\partial x^a} \frac{\partial g}{\partial p_a} - \frac{\partial f}{\partial p_a} \frac{\partial g}{\partial x^a} \right), \tag{1.1}$$

in particular, $\{x^a, p_b\} = \delta^a_b$. All local physical quantities (classical observables) f are real functions of the phase-space variables, $f = f(x, p)$. Classical observables form a real associative commutative algebra, in particular, $[f_1, f_2] \equiv f_1 f_2 - f_2 f_1 = 0$, $\forall f_1, f_2$.

(b) In QM, a state of a physical system at any instant of time is specified by a vector ψ in a Hilbert space $\mathfrak{H}$, which is called the space of states. A scalar product of two vectors ψ_1 and ψ_2 is denoted by (ψ_1, ψ_2). To a first approximation, it is assumed that any state $\psi \in \mathfrak{H}$ can be realized physically; in particular, the superposition principle holds: if states ψ_1 and ψ_2 are realizable, then the state $\psi = a_1\psi_1 + a_2\psi_2$ with any $a_1, a_2 \in \mathbb{C}$ is also realizable.

(c) In QT, each classical observable $f = f(x, p)$ is assigned an s.a. operator $\hat{f}$, $f \longmapsto \hat{f}$, acting in a Hilbert space $\mathfrak{H}$. It is called a quantum observable. To a first approximation, it is assumed that any operator $\hat{f}$, including observables, is defined on any state ψ, i.e., $\hat{f}\psi \in \mathfrak{H}$, $\forall \psi \in \mathfrak{H}$, and is uniquely determined by its matrix elements $\left(\psi_1, \hat{f}\psi_2\right)$, $\forall \psi_1, \psi_2 \in \mathfrak{H}$, and what is more, by its matrix $f_{mn} = (e_m, \hat{f} e_n)$ with respect to any orthonormal basis $\{e_n\}_1^\infty$, a complete orthonormalized set of vectors in $\mathfrak{H}$. Then any operator $\hat{f}$ is assigned its adjoint $\hat{f}^+$ defined by

$$\left(\psi_1, \hat{f}^+\psi_2\right) = \left(\hat{f}\psi_1, \psi_2\right), \ \forall \psi_1, \psi_2 \in \mathfrak{H},$$

and thereby the involution (conjugation) $\hat{f} \longmapsto \hat{f}^+$ is defined in the algebra of operators with the properties[6]

$$\left(\hat{f}^+\right)^+ = \hat{f}, \ \left(a\hat{f}\right)^+ = \overline{a}\hat{f}^+, \ \forall a \in \mathbb{C},$$

$$\left(\hat{f} + \hat{g}\right)^+ = \hat{f}^+ + \hat{g}^+, \ \left(\hat{f}\hat{g}\right)^+ = \hat{g}^+\hat{f}^+.$$

The self-adjointness of $\hat{f}$ means that $\hat{f} = \hat{f}^+$, or

$$\left(\psi_1, \hat{f}\psi_2\right) = \left(\hat{f}\psi_1, \psi_2\right), \ \forall \psi_1, \psi_2 \in \mathfrak{H}.$$

[6]The bar $^-$ over an expression denotes complex conjugation.

The mean value $\langle \hat{f} \rangle_\psi$ of any quantum observable $\hat{f}$ in a state ψ and the corresponding dispersion Δf are respectively defined by

$$\left\langle \hat{f} \right\rangle_\psi = \frac{\left(\psi, \hat{f}\psi\right)}{(\psi, \psi)},$$
$$\Delta f = \sqrt{\left\langle \left(\hat{f} - \langle \hat{f} \rangle_\psi\right)^2 \right\rangle_\psi} = \sqrt{\left\langle \hat{f}^2 \right\rangle_\psi - \left\langle \hat{f} \right\rangle_\psi^2}.$$

The self-adjointness of observables is assumed to imply that any observable $\hat{f}$ can be diagonalized, which means that the eigenvectors, or eigenstates, of $\hat{f}$ form an orthonormal basis in $\mathfrak{H}$; the spectrum of an observable is defined as a set of all its eigenvalues. The spectrum determines possible measurable values of the corresponding observable, while the complete orthonormalized set of the eigenstates of the observable provides a probabilistic interpretation of its measurements.

(d) According to the correspondence principle, there exists a certain relation between the Poisson bracket $\{f_1, f_2\} = f_3$ of classical observables f_1 and f_2 and the commutator $[\hat{f}_1, \hat{f}_2]$ of their quantum counterparts $\hat{f}_1$ and $\hat{f}_2$, namely, $[\hat{f}_1, \hat{f}_2] = i\hbar \hat{f}_3 + \hat{O}\left(\hbar^2\right)$; a supplementary operator $\hat{O}\left(\hbar^2\right)$ vanishes with vanishing $\hbar$ as $\hbar^2$. A more transparent form can be given to this correspondence:

$$\{f_1, f_2\} \longrightarrow \frac{1}{i\hbar}\left[\hat{f}_1, \hat{f}_2\right] + \hat{O}(\hbar).$$

That is, according to the correspondence principle, the Poisson bracket of classical observables is assigned the commutator of their quantum counterparts times the factor $(i\hbar)^{-1}$ plus, in general, a supplementary operator $\hat{O}(\hbar)$.

The position operators $\hat{x}^a$ and momentum operators $\hat{p}^a$ are postulated to be s.a. and satisfy the canonical commutation relations

$$\left[\hat{x}^a, \hat{x}^b\right] = \left[\hat{p}_a, \hat{p}_b\right] = 0, \ \left[\hat{x}^a, \hat{p}_b\right] = i\hbar\left\{x^a, p_b\right\} = i\hbar\delta^a_b. \tag{1.2}$$

The correspondence principle requires that the quantum counterpart $\hat{f}$ of a classical observable $f(x, p)$ be of the form $\hat{f} = f(\hat{x}, \hat{p}) + \hat{O}(\hbar)$. A supplementary operator $\hat{O}(\hbar)$ is generally necessary to provide the self-adjointness of $\hat{f}$. In the general case, the correspondence principle does not allow a unique construction of the operator function $f(\hat{x}, \hat{p})$ in terms of the classical function $f(x, p)$ because of the noncommutativity of $\hat{x}$ and $\hat{p}$ (the so-called ordering problem.[7])

[7]Numerous papers have been devoted to the study of various rules of assigning operators to classical quantities. A substantial contribution to a resolution of this problem is due to Berezin [25].

To the first approximation whereby any observable can be diagonalized, it is argued that commuting observables $\hat{f}_1$ and $\hat{f}_2$ have a joint spectrum, i.e., a common set of eigenvectors, which implies the simultaneous measurability of the observables. A complete set of observables is defined as a minimum set of n commuting observables $\hat{f}_k, \ \ k = 1, \ldots, n$, $[\hat{f}_k, \hat{f}_l] = 0, \ \forall k, l$, whose joint spectrum is nondegenerate and whose common eigenvectors provide a unique specification of any vector in terms of the corresponding expansion with respect to these eigenvectors. For a complete set of observables, we can choose all the position operators $\hat{x}^a$. The momentum operators $\hat{p}_a$ can also be chosen for a complete set of observables. Different complete sets of observables can be considered, and their spectrum and eigenvectors specify the quantum description of a system under consideration.

(e) The time evolution of a state of the system in the course of time t is described by the Schrödinger equation for the state vector $\psi(t)$,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi, \tag{1.3}$$

with an initial condition $\psi(t_0) = \psi_0$, where the operator $\hat{H}$, the quantum Hamiltonian, the energy observable, corresponds to the classical Hamiltonian H.

Because the initial state ψ_0 can be arbitrary, it is assumed that $\hat{H}$ is certainly applicable to any state $\psi \in \mathfrak{H}$.

A realization of the canonical commutation relations (1.2) in a specific Hilbert space (representation of canonical commutation relations) offers a practical possibility for solving the Schrödinger equation and finding probabilities of transitions from one state to another, means of physical quantities, and probabilities of measurements using the accepted rules.

It was canonical quantization that was first used to construct the QT for the simplest systems. There exist alternative formulations of QT, for example formulations in terms of Green's functions, functional integrals, and so on. Each of these formulations can either be introduced independently by a set of postulates or "derived" logically from the operator formulation based on the canonical quantization method. In the latter case, an alternative formulation of QT for a specific system is said to be obtained by the canonical quantization method. It should be noted that among all the formulations, the operator formulation based on canonical quantization is the best-developed and most consistent one. This explains the existing tendency to quantize every classical system canonically. We should note that for classical systems of general form, canonical quantization is not always possible or cannot be carried out directly as described above without an essential analysis and reformulation of the initial classical theory. The majority of modern physical theories belong to the so-called singular theories, theories with constraints and extra nonphysical variables in the initial Hamiltonian formulation (gauge theories are a particular case of singular theories). There exist different methods for quantizing such theories; see, e.g., [49, 75, 91]. Some of these methods are based on the possibility of passing to physical variables, which allows the standard canonical quantization. Canonical quantization remains the most reliable quantization scheme.

1.3 Some Paradoxes of Naïve Implementation of an Idealized Scheme

In this section, we examine some simple QM systems obtained in the framework of the above-described idealized scheme of operator canonical quantization. We show that if we follow this scheme literally, we arrive at certain paradoxes in the form of obvious contradictions with well-known statements.

We consider an example of a very simple system: a free nonrelativistic particle of mass m moving on an interval (a, b) of the real axis. The interval can be finite or infinite, a semiaxis or the whole axis. The finite ends of an interval are considered to be included in the interval; in particular, by a finite interval, we mean a closed interval $[a, b]$.

In classical mechanics, the phase space of this system is a strip $(a, b) \times \mathbb{R}$; the ranges of the particle position x and momentum p are respectively (a, b) and $\mathbb{R}$. The Poisson bracket (1.1) of x and p is $\{x, p\} = 1$. Free motion is defined by the free Hamiltonian $\mathcal{H} = p^2/2m$. If $|a| < \infty$ and/or $|b| < \infty$, the peculiarity of the system is that its phase space is a space with boundaries. The behavior of the particle near the boundaries must be specified by some subsidiary conditions such as elastic reflection, delay, trapping, or something else.

At first glance, we may not face the problem of boundaries when quantizing this system. The canonical observables for a QM particle are the position operator $\hat{x}$ and the momentum operator $\hat{p}$ satisfying the canonical commutation relations

$$[\hat{x}, \hat{x}] = [\hat{p}, \hat{p}] = 0, \ \ [\hat{x}, \hat{p}] = i\hbar\{x, p\} = i\hbar. \tag{1.4}$$

For a complete set of observables, we can take the position operator $\hat{x}$ with the prescription that its spectrum be given by spec $\hat{x} = (a, b)$. It is natural to take the x-representation of canonical commutation relations (1.4) where the Hilbert space $\mathfrak{H}$ of states is the space of functions $\psi(x)$ square-integrable on the interval (a, b); $\mathfrak{H} = L^2(a, b)$; the operator $\hat{x}$ is the operator of multiplication by x, namely

$$\hat{x}\psi(x) = x\psi(x);$$

while the operator $\hat{p}$ is a multiple of the differentiation operator[8] $d_x = \mathrm{d}/\mathrm{d}x$:

$$\hat{p} = -i\hbar d_x : \; \hat{p}\psi(x) = -i\hbar\psi'(x).$$

The canonical commutation relations (1.4) seem obviously to hold.

Other observables are certain differential operators

$$\hat{f} = f(x, -i\hbar d_x) + O(\hbar).$$

In particular, the free quantum Hamiltonian is given by

$$\widehat{\mathcal{H}} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} d_x^2. \tag{1.5}$$

All this appears quite natural from the following standpoint as well. If $|a| < \infty$ and/or $|b| < \infty$, the space $L^2(a,b)$ can be considered the subspace of functions vanishing outside the interval (a,b) in the space $L^2(\mathbb{R})$ of states of a particle on the whole real axis $\mathbb{R}$, whereas all the observables defined on $L^2(a,b)$, including $\hat{x}$ and $\hat{p}$, can be considered restrictions to this subspace of well-known s.a. operators defined on $L^2(\mathbb{R})$. For the case of a finite interval $[a,b]$, the position operator $\hat{x}$ becomes a bounded s.a. operator defined everywhere. Considering $\hat{p}$ as an s.a. operator, we have a set of three s.a. operators $\hat{x}$, $\hat{p}$, and $\widehat{\mathcal{H}}$ with the commutation relations

$$[\hat{x}, \hat{p}] = i\hbar, \; \left[\hat{p}, \widehat{\mathcal{H}}\right] = 0. \tag{1.6}$$

If all the previous statements hold, then the following observations seem paradoxical and cast doubt on the consistency of the adopted quantization scheme.

1.3.1 Paradox 1

Let $\psi_p(x)$ be an eigenvector of the s.a. momentum operator, $\hat{p}\psi_p = p\psi_p$. Based on the self-adjointness of the operators $\hat{p}$ and $\hat{x}$, we have the chain of equalities

$$\begin{aligned}\left(\psi_p, [\hat{x}, \hat{p}]\psi_p\right) &= \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\psi_p, \hat{p}\hat{x}\psi_p\right) \\ &= p\left(\psi_p, \hat{x}\psi_p\right) - \left(\hat{p}\psi_p, \hat{x}\psi_p\right) \\ &= p\left[\left(\psi_p, \hat{x}\psi_p\right) - \left(\psi_p, \hat{x}\psi_p\right)\right] = 0,\end{aligned}$$

which obviously contradicts the commutation relation (1.6).

[8] It is rather a differential operation than a differential operator; see Chap. 4. A rigorous definition of the differentiation operator $\hat{d}_x$ is given in the end of Sect. 2.3.4.

In addition, this commutation relation implies the well-known Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}\,, \tag{1.7}$$

where Δx and Δp are the respective dispersions of the position and momentum for any state ψ of a particle. But for the case of a finite interval $[a, b]$ and for $\psi = \psi_p$, we have $\Delta x \leq b - a$, $\Delta p = 0$, and therefore $\Delta x \Delta p = 0$, which contradicts (1.7).

An explanation of the above paradoxes is given in Chap. 6. It is different for different types of interval: depending on the type of interval, either an s.a. momentum operator does not exist, or it exists but has no eigenvectors, or even if such vectors exist, they do not belong to the domain of the operator $\hat{p}\hat{x}$. In addition, in the case of a semiaxis or a finite interval, the canonical commutation relations together with the uncertainty principle do not hold.

1.3.2 Paradox 2

We now consider a free particle moving on a finite interval $[0, l]$. If we treat a motion governed by the Hamiltonian (1.5) as a motion in an infinite rectangular potential well, then the eigenvalues of the Hamiltonian and the corresponding eigenfunctions are well known from any textbook:

$$\widehat{\mathcal{H}}\psi_n(x) = E_n\psi_n(x)\,, \quad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{l}\right)^2 n^2, \tag{1.8}$$

$$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{\pi n}{l}x\right), \quad n \in \mathbb{N}. \tag{1.9}$$

The set $\{\psi_n(x)\}_1^\infty$ of these eigenfunctions is an orthonormal basis in $L^2(0, l)$, which confirms the self-adjointness of the Hamiltonian.

As is also well known, two commuting s.a. operators have common eigenvectors, and if the spectrum of one of the commuting s.a. operators is nondegenerate, then its eigenvectors must be eigenvectors of another s.a. operator. In our case, we have two commuting s.a. operators $\hat{p}$ and $\widehat{\mathcal{H}}$, and the spectrum (1.8) of $\widehat{\mathcal{H}}$ is nondegenerate. Therefore, eigenfunctions (1.9) must be the eigenfunctions of $\hat{p}$. But we have

$$\hat{p}\psi_n(x) = -i\hbar\sqrt{\frac{2}{l}}\frac{\pi n}{l}\cos\frac{\pi n}{l}x \neq p_n\psi_n(x)$$

for any n, which contradicts the above assertion.

As explained in Chap. 6, this paradox is a consequence of the incorrect assumption that $\hat{p}$ and $\widehat{\mathcal{H}}$ commute; in particular, it is a consequence of the naïve belief that the Hamiltonian $\widehat{\mathcal{H}}$ can be represented as $\widehat{\mathcal{H}} = \hat{p}^2/2m$.

1.3.3 Paradox 3

As mentioned above, in standard textbooks on QM for physicists, some important notions related to operators in Hilbert spaces are often introduced in terms of their matrix elements with respect to an orthonormal basis, because it is believed that the matrix elements $f_{mn} = (e_m, \hat{f} e_n)$ of an operator $\hat{f}$ with respect to an orthonormal basis $\{e_n\}_1^\infty$ completely determine the operator $\hat{f}$ according to the following chain of equalities:

$$\psi = \sum_{n=1}^{\infty} \psi_n e_n, \; \psi_n = (e_n, \psi), \; \hat{f} e_n = \sum_{m=1}^{\infty} f_{mn} e_m,$$
$$\hat{f}\psi = \sum_{n=1}^{\infty} \psi_n \hat{f} e_n = \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} f_{mn} \psi_n \right) e_m.$$

For example, the adjoint $\hat{f}^+$ of $\hat{f}$ is defined as an operator whose matrix elements are given by

$$(f^+)_{mn} = \left(e_m, \hat{f}^+ e_n \right) = \left(\hat{f} e_m, e_n \right) = \overline{\left(e_n, \hat{f} e_m \right)} = \overline{f_{nm}}.$$

Correspondingly, an s.a. operator $\hat{f} = \hat{f}^+$ is defined as an operator whose matrix is Hermitian $f_{mn} = \overline{f_{nm}}$.

But let us consider the matrix $p_{mn} = (e_m, \hat{p} e_n)$ of the momentum operator $\hat{p}$ in the Hilbert space $L^2(0, l)$ with respect to the orthonormal basis $\{e_n\}_0^\infty$,

$$e_n(x) = \sqrt{\frac{2}{l}} \cos\left(\frac{\pi n}{l} x \right), \; n \in \mathbb{R}_+. \tag{1.10}$$

A direct calculation by integrating by parts shows that

$$\overline{p_{nm}} = p_{mn} + i\left[e_m(l) e_n(l) - e_m(0) e_n(0) \right] \neq p_{mn}, \; m + n = 2k + 1, \tag{1.11}$$

i.e., the matrix p_{mn} is not Hermitian, contrary to our expectations.

As is explained in Chap. 6, the paradox is related to the fact that the orthonormal basis (1.10) does not belong to the domain of any s.a. operator $\hat{p}$ from the whole family of admissible momentum operators.

1.3.4 Paradox 4

Let us consider a free particle on a segment $[0, l]$ as a particle in an infinite rectangular potential well, and let us calculate the mean of the squared energy $\langle E^2 \rangle$ for the state given by the wave function

$$\psi(x) = Nx(x-l), \tag{1.12}$$

where N is a normalization factor. Because $\left(\widehat{\mathcal{H}}\right)^2 \psi = 0$, this mean must be zero:

$$\langle E^2 \rangle = \left(\psi, \left(\widehat{\mathcal{H}}\right)^2 \psi\right) = 0.$$

On the other hand, using the self-adjointness of $\widehat{\mathcal{H}}$, we obtain a nonzero result for the same quantity:

$$\langle E^2 \rangle = \left(\widehat{\mathcal{H}}\psi, \widehat{\mathcal{H}}\psi\right) = \frac{N^2\hbar^4 l}{m^2}.$$

As explained in Chap. 6, a solution of the paradox is related to the fact that the function $\widehat{\mathcal{H}}\psi(x)$ does not belong to the domain of a correctly defined Hamiltonian $\widehat{\mathcal{H}}$ associated with an infinite potential well, although the function $\psi(x)$ does.

1.3.5 Paradox 5

We consider the Schrödinger equation for a free particle on the segment $[0, l]$,

$$i\hbar\frac{\partial\psi(t,x)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(t,x), \ x \in [0,l]. \tag{1.13}$$

We recall that in the idealized quantization scheme, the time-evolution problem in the form (1.13) can be posed for an arbitrary initial state. Let the initial state $\psi_0(x) = \psi(t_0, x)$ at $t_0 = 0$ be

$$\psi(0,x) = C\exp\left(\frac{\mathrm{i}+1}{\sqrt{2}}\frac{kx}{\hbar}\right), \tag{1.14}$$

where k is a fixed real parameter with dimension of momentum. It is easy to verify that the solution $\psi(t, x)$ of (1.13) with initial condition (1.14) is given by

$$\psi(t,x) = \exp\left(-\frac{k^2}{2m\hbar}t\right)\psi_0(x). \tag{1.15}$$

It is surprising that the evolution of the given initial state is not unitary: the wave function $\psi(t, x)$ "vanishes" with time. This situation is evidently related to the fact that formally, we have

$$\widehat{\mathcal{H}}\psi_0(x) = -\frac{ik^2}{2m}\psi_0(x) \Longrightarrow \widehat{\mathcal{H}}\psi(t,x) = -\frac{ik^2}{2m}\psi(t,x),$$

i.e., the initial state ψ_0 and the evolving state $\psi(t)$ are the eigenstates of the s.a. Hamiltonian with a pure imaginary eigenvalue, which is impossible, as is well known.

As explained in Chap. 6, a resolution of the paradox lies in the fact that if the function $\psi_0(x)$ does not belong to the domain of any correctly defined s.a. Hamiltonian $\widehat{\mathcal{H}}$ from the whole family of admissible Hamiltonians for a free particle on the interval $[0, l]$, then $\psi(t, x)$ also does not, which is irreconcilable with the Schrödinger equation.

1.3.6 Concluding Remarks

In the foregoing, we discussed some QM paradoxes arising under a naïve treatment of simple one-dimensional systems with boundaries. The number of paradoxes can be extended (see, for example, [31, 74]), and certain of the others are examined below. In Chap. 7, we discuss possible paradoxes related to singular potentials with a simple example of a particle moving on the real axis or a semiaxis in the so-called Calogero potential field $V(x) = \alpha/x^2$. But even the above examples seem to be sufficient to convince the reader–physicist that a rigorous approach to the definition of operators and especially of observables in QM is a necessity. The point is that up to now, we were too naïve in our analysis; strictly speaking, our arguments were incorrect, and our conclusions were wrong. The reason is that all the operators involved are unbounded, and for unbounded operators, the algebraic rules and the notion of commutativity are nontrivial. In fact, the above-used rules and notions were uncritically borrowed from finite-dimensional algebra; they are valid for bounded operators, while for unbounded operators, a special treatment is necessary. The correct treatment removes all the paradoxes.

Chapter 2
Linear Operators in Hilbert Spaces

In this chapter, we remind the reader of basic notions and facts from the theory of Hilbert spaces and of linear operators in such spaces which are relevant to the subject of the present book.

2.1 Hilbert Spaces

2.1.1 Definitions and General Remarks

Definition 2.1. (A) A *Hilbert space* $\mathfrak{H}$ is a linear space over the complex numbers. As a rule, the elements of $\mathfrak{H}$ (vectors or points) are denoted by Greek letters: $\xi, \eta, \zeta, \varphi, \psi, \chi, \ldots \in \mathfrak{H}$, whereas numbers, complex or real, are denoted by italic Latin letters: $a, b, c, x, y, z, \ldots \in \mathbb{C}$ or $\mathbb{R}$. In what follows, we consider infinite-dimensional Hilbert spaces.[1]

(B) The space $\mathfrak{H}$ is endowed with a scalar product that is a positive definite sesquilinear form on $\mathfrak{H}$. This means that every pair of vectors ξ, η is assigned a complex number (ξ, η), the scalar product of ξ and η, with the properties[2]

$$(\xi, \eta) = \overline{(\eta, \xi)}\,;\ (\xi, \xi) \geq 0\,,\ \text{and}\,(\xi, \xi) = 0\ \text{iff}\ \xi = 0\,;$$

$$(\xi, a\zeta + b\eta) = a(\xi, \zeta) + b(\xi, \eta) \Longrightarrow (a\xi + b\zeta, \eta) = \overline{a}(\xi, \eta) + \overline{b}(\zeta, \eta)\,.$$

[1] Finite-dimensional Hilbert spaces (or Euclidean spaces) are also encountered in QM as spaces of states, e.g., in QM of two-level systems, finite spin systems, and so on. Finite-dimensional spaces are free from the problems that are examined in the present book.

[2] We use "iff" in its standard usage for "if and only if." For brevity, the arrow $\Longrightarrow$ stands for "implies."

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The nonnegative arithmetic square root $\sqrt{(\xi,\xi)}$ is called the norm, or length, of a vector ξ, and is denoted by $\|\xi\|$, $\|\xi\| = \sqrt{(\xi,\xi)}$. A vector ξ is called normalized if $\|\xi\| = 1$. Any nonzero vector ξ can be normed: $\xi \longmapsto \xi^{\mathrm{n}} = \xi/\|\xi\|$. For any two vectors ξ and η, the *Cauchy–Schwarz inequality* (also known as the Cauchy–Bunyakovskii inequality) $|(\xi,\eta)| \leq \|\xi\|\|\eta\|$ holds. A corollary of the Cauchy–Schwarz inequality is the triangle inequality $\|\xi + \eta\| \leq \|\xi\| + \|\eta\|$ for the norm.

The distance between two points ξ and η is defined as $\|\xi - \eta\|$. The triangle inequality for the distance becomes $\|\xi - \eta\| \leq \|\xi - \zeta\| + \|\eta - \zeta\|$.

The distance determines a topology[3] in $\mathfrak{H}$. A sequence $\{\xi_n\}_1^\infty$ of vectors is said to be convergent to a vector ξ, or equivalently, we say that ξ is the limit of this sequence, written $\xi_n \to \xi$, $n \to \infty$, or $\xi = \lim_{n\to\infty} \xi_n$, if $\|\xi_n - \xi\| \to 0$, $n \to \infty$. Because of the triangle inequality, a necessary condition for convergence is

$$\|\xi_m - \xi_n\| \to 0, \;\; m, n \to \infty. \tag{2.1}$$

A sequence $\{\xi_n\}_1^\infty$ with property (2.1) is called a fundamental sequence or a Cauchy sequence.

Linear operations in $\mathfrak{H}$ (multiplication of vectors by complex numbers and vector addition) and the scalar product are continuous in their arguments; for example,

$$\xi_n \to \xi \Rightarrow (\xi_n, \eta) \to (\xi, \eta), \;\; \forall \eta \in \mathfrak{H},$$

because of the Cauchy–Schwarz inequality.

A set $M \subset \mathfrak{H}$ is said to be dense in $\mathfrak{H}$ if any vector in $\mathfrak{H}$ can be approximated by vectors belonging to M with any desired accuracy, i.e., if for any $\xi \in \mathfrak{H}$, there exists a sequence $\{\xi_n\}_1^\infty$, $\xi_n \in M$, so that $\xi = \lim_{n\to\infty} \xi_n$.

(C) $\mathfrak{H}$ is complete**.** This means that every Cauchy sequence $\{\xi_n\}_1^\infty$ in $\mathfrak{H}$ is convergent, or has a limit in $\mathfrak{H}$:

$$\|\xi_m - \xi_n\| \to 0, \; m, n \to \infty \Rightarrow \exists \xi \in \mathfrak{H} : \xi_n \to \xi, \; n \to \infty.$$

As mentioned above, any convergent sequence $\{\xi_n\}_1^\infty$ is a Cauchy sequence. In a Hilbert space, the converse also holds.[4] A space satisfying requirements (A) and (B) is called a pre-Hilbert space. Any pre-Hilbert space can be made a complete Hilbert space by adding the "limits" of Cauchy sequences.

We note that the requirement of completeness is crucial, and not only technical, for applications of Hilbert spaces to QM.

(D) A Hilbert space $\mathfrak{H}$ is called separable if it contains a countable dense set.

[3]A Hilbert space is a particular case of a normed and metric space in which a norm and a metric (distance) satisfying standard requirements are generated by a scalar product; see [9].

[4]In short, a Hilbert space is complete with respect to a metric generated by a scalar product.

Separable Hilbert spaces are sufficient for treating conventional QM, and we here restrict ourselves to separable Hilbert spaces. We return to the notions of dense set and separability below.

An example of a Hilbert space is the space l^2 of sequences $\xi = \{x_n\}_1^\infty$ of complex numbers such that the sum of their moduli squared is convergent,

$$l^2 = \left\{ \xi = \{x_n\}_1^\infty \,,\ x_n \in \mathbb{C} : \sum_{i=1}^{\infty} |x_n|^2 < \infty \right\}.$$

The numbers x_n are called the components of a vector ξ. Linear operations are defined via components: if $\xi = \{x_n\}_1^\infty$ and $\eta = \{y_n\}_1^\infty$, then $a\xi + b\eta = \{ax_n + by_n\}_1^\infty$. The scalar product of vectors ξ and η is defined by $(\xi, \eta) = \sum_{i=1}^\infty \overline{x_n} y_n$. The correctness of the definition and the completeness of l^2 are easily verified.

A vector ξ is called terminating if it has a finite number of nonzero components. The set of all terminating vectors is a dense subspace in l^2. A Euclidean space of arbitrary dimension is naturally embedded in l^2 as a subspace. The Hilbert space l^2 is separable: a countable dense set in l^2 is the set of terminating vectors whose components are complex numbers with rational real and imaginary parts.

2.1.2 *Elements of Geometry and Topology*

By an ε-neighborhood of a point ξ_0 we mean an open ball $B_{\varepsilon,\xi_0} = \{\xi : \|\xi - \xi_0\| < \varepsilon\}$. A point ξ is called an interior point of a set $M \subset \mathfrak{H}$ if it belongs to M together with an ε-neighborhood of ξ. A set $M \subset \mathfrak{H}$ is called an open set if all of its points are interior. A set $M \subset \mathfrak{H}$ is called a bounded set if $M \subset B_{r,0}$ for some $r > 0$.

A point ξ is called a limit point of a set $M \subset \mathfrak{H}$ if in any neighborhood of ξ, there exists an infinite number of points belonging to M. An equivalent definition of a limit point is this: a vector ξ is a limit point of a set M if there exists a sequence $\{\xi_n\}_1^\infty$, $\xi_n \in M$, so that $\xi = \lim_{n\to\infty} \xi_n$. A set M is said to be closed if it contains all of its limit points, which is denoted by $M = \overline{M}$. The complement $\mathfrak{H} \setminus M$ of an open set M in $\mathfrak{H}$ is closed.

Any set $M \subset \mathfrak{H}$ can be made closed by adding all of its limit points. We call this operation the closure operation and denote the closure of a set M by $\overline{M}$.[5] It is evident that $M \subseteq \overline{M}$; equality holds for a closed set M, and $\overline{M}$ is the minimal closed set containing M.

Returning to the notion of a dense set, we can now say that a set $M \subset \mathfrak{H}$ is said to be dense (in $\mathfrak{H}$) if $\overline{M} = \mathfrak{H}$, i.e., if its closure coincides with the whole space.

[5]We hope that there will be no confusion with the similar symbols for complex conjugation and closure; they refer to different notions, the first involving complex numbers, and the second, sets.

In connection with QM, the sets in $\mathfrak{H}$ that are linear spaces in themselves, i.e., are invariant under linear operations, are of special importance. A set that is a linear space is called a subspace and is usually denoted by D:

$$D = \{\xi : \xi, \eta \in D \Longrightarrow a\xi + b\eta \in D, \ \forall a, b \in \mathbb{C}\} \subseteq \mathfrak{H}.$$

It is evident that in any subspace D, there exists an induced scalar product that is the restriction of the original scalar product in $\mathfrak{H}$ to D. If D is finite-dimensional, then it is a Euclidean space, which is always closed and complete. If D is infinite-dimensional, it is at least a pre-Hilbert space. If such a D is closed, $D = \overline{D}$, then D itself is a Hilbert space.

The simplest example of a subspace is the linear envelope $L(\{\xi_n\}_1^N)$ of a sequence of vectors $\{\xi_n\}_1^N$ (N can be infinite). This is the set of all finite linear combinations of vectors in $\{\xi_n\}_1^N$:

$$L\left(\{\xi_n\}_1^N\right) = \{\xi : \xi = a_{n_1}\xi_{n_1} + \cdots + a_{n_k}\xi_{n_k}\,, \ \forall k \leq N\}.$$

Equality in the last inequality is possible only if $N < \infty$.

If $L\left(\{\xi_n\}_1^\infty\right)$ is dense, the sequence $\{\xi_n\}_1^\infty$ is called a complete sequence.

The criteria for D to be dense and for $\{\xi_n\}_1^\infty$ to be complete are formulated in terms of orthogonality. The notions of orthogonality and orthogonal decomposition are of primary importance for QM.

Two vectors ξ and η are called orthogonal, and we write $\xi \perp \eta$, if $(\xi, \eta) = 0$. A sequence $\{e_n\}_1^N$ (N can be infinite) is called an orthonormalized sequence if $(e_k, e_l) = \delta_{\mathrm{kl}}$, where δ_{kl} is the Kronecker symbol. In a separable Hilbert space, any orthonormalized sequence of vectors is a finite or countable set. A proof of this fact can be found in [9, 116]. A similar assertion is easily extended to sequences of nonzero orthogonal vectors.

Any sequence $\{\xi_n\}_1^N$ (N can be infinite) can be orthonormalized (by the Gram–Schmidt orthogonalization procedure). This means that there exists an orthonormalized sequence $\{e_n\}_1^N$ equivalent to $\{\xi_n\}_1^N$ in the sense that $L(\{\xi_n\}_1^N) = L(\{e_n\}_1^N)$. A complete orthonormalized sequence $\{e_n\}_1^\infty$ is called a (countable) orthonormal basis in $\mathfrak{H}$, or simply an orthonormal basis. A Hilbert space $\mathfrak{H}$ is separable iff it has a countable orthonormal basis $\{e_n\}_1^\infty$.

A vector η is called orthogonal to a set $M \subset \mathfrak{H}$, and we write $\eta \perp M$, if $\eta \perp \xi$, $\forall \xi \in M$. The notion of orthogonality is naturally extended to any number of sets. The set of all vectors orthogonal to a given subspace D is called the orthogonal complement of D and is denoted by $D^\perp$, $D^\perp = \{\eta : \eta \perp D\}$. By definition, $D \perp D^\perp$.

We call the operation $^\perp$ that assigns the orthogonal complement $D^\perp$ to each subspace D, $D \xrightarrow{\perp} D^\perp$, the orthogonal complement operation.

It is evident that $D^\perp$ is a linear space and moreover is a closed subspace coinciding with $\overline{D}^\perp$,

$$D^\perp = \overline{D^\perp} = \overline{D}^\perp, \tag{2.2}$$

because of the continuity of the scalar product in both arguments; in other words, the orthogonal complement of any subspace is closed, the closure operation $^{-}$ and the orthogonal complement operation $^{\perp}$ commute, and the orthogonal complements of a subspace and of its closure are the same. It is evident that the orthogonal complement of the whole of $\mathfrak{H}$ is the zero subspace $\{0\}$: $(\eta, \xi) = 0, \ \forall \xi \in \mathfrak{H} \Longrightarrow \eta = 0$; it is sufficient to take $\xi = \eta$.

It is also evident that

$$D_1 \subseteq D_2 \Longrightarrow D_1^{\perp} \supseteq D_2^{\perp}. \tag{2.3}$$

Before we proceed further, we recall the notions of direct sum in the theory of linear spaces. Let L_1 and L_2 be subspaces in a linear space L. We call L the direct sum of L_1 and L_2, and write

$$L = L_1 + L_2$$

if

$$\xi = \xi_1 + \xi_2 \in L \ , \ \ \forall \xi_1 \in L_1 \ , \ \ \forall \xi_2 \in L,$$

and any $\xi \in L$ is uniquely represented as $\xi = \xi_1 + \xi_2, \xi_1 \in L_1, \xi_2 \in L_2$. A necessary condition for the equality $L = L_1 + L_2$ is $L_1 \cap L_2 = \{0\}$. Conversely, if L_1 and L_2 do not intersect except at zero, $L_1 \cap L_2 = \{0\}$, we can construct the direct sum

$$L = L_1 + L_2 = \{\xi : \ \xi_1 + \xi_2, \ \ \forall \xi_1 \in L_1, \ \ \forall \xi_2 \in L_2\}.$$

By induction, the notion of a direct sum is extended to any number of summands.

Moreover, we can construct a direct sum of two linear spaces that are not subspaces of the same linear space. Let L_1 and L_2 be linear spaces (L_2 can be a copy of L_1). Then their direct sum $L = L_1 + L_2$ is the set of all ordered pairs ξ_1, ξ_2, where $\xi_1 \in L_1$ and $\xi_2 \in L_2$. These pairs are conveniently written as columns[6] (ξ_1 / ξ_2), so that $L = L_1 + L_2 = \{(\xi_1 / \xi_2), \forall \xi_1 \in L_1, \forall \xi_2 \in L_2\}$. Linear operations in L are defined componentwise.

In Hilbert spaces, there exists an additional structure of a direct sum associated with a possible orthogonality of summands. Let $D = D_1 + D_2$ and let $D_1 \perp D_2$. Then the direct sum is called the orthogonal direct sum. For such a sum, we use the sgn $\oplus$, $D = D_1 \oplus D_2$. This equality is equivalent to each of the equalities $D_1 = D \ominus D_2$ and $D_2 = D \ominus D_1$. The notion of an orthogonal direct sum is easily extended to any number of mutually orthogonal subspaces:

$$D = \sum_k{}^{\oplus} D_k \ , \ \ D_k \perp D_l \ , \ \ k \neq l \ , \ \ \forall k, l.$$

[6]We are forced to use the symbol (ξ_1 / ξ_2) for a two-component column ("spinor") instead of the conventional symbol $\begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$ for reasons of space.

We call the operation $\oplus$ of taking the orthogonal direct sum of (sub)spaces, $D_1, D_2 \xrightarrow{\oplus} D_1 \oplus D_2$, the orthogonal direct sum operation.

A useful construction for defining and studying linear operators in a Hilbert space $\mathfrak{H}$ is the Hilbert space $\mathbb{H}=\mathfrak{H} \oplus \mathfrak{H}$, the orthogonal direct sum of two copies of $\mathfrak{H}$. Elements Ψ of $\mathbb{H}$ (vectors) are ordered pairs $\xi, \eta \in \mathfrak{H}$ arranged in columns, $\Psi = (\xi/\eta)$, where ξ is the upper component and η is the lower component:

$$\mathbb{H} = \mathfrak{H} \oplus \mathfrak{H} = \{\Psi = (\xi/\eta)\,,\ \forall \xi, \eta \in \mathfrak{H}\}.$$

Linear operations in $\mathbb{H}$ are conventionally defined via components; the scalar product is defined by $(\Psi_1, \Psi_2) = (\xi_1, \xi_2) + (\eta_1, \eta_2)$.

We now can cite a theorem on projection onto a closed subspace [9].

Theorem 2.2. *Let D be a closed subspace of a Hilbert space $\mathfrak{H}$, $D = \overline{D} \subseteq \mathfrak{H}$, and let $D^{\perp}$ denote its orthogonal complement, $D^{\perp} = \overline{D^{\perp}} \subseteq \mathfrak{H}$, $D^{\perp} \perp D$.*

For any D, the Hilbert space $\mathfrak{H}$ is decomposed into the orthogonal direct sum of D and $D^{\perp}$,

$$\mathfrak{H} = D \oplus D^{\perp}, \tag{2.4}$$

which means that any vector $\xi \in \mathfrak{H}$ is uniquely represented as

$$\xi = \xi_{\|} + \xi_{\perp},\ \xi_{\|} \in D,\ \xi_{\perp} \in D^{\perp},\ (\xi_{\|}, \xi_{\perp}) = 0; \tag{2.5}$$

the vector $\xi_{\|}$ is called the projection of ξ on D.

The orthogonal decomposition (2.4) has a number of corollaries.

Corollary 2.3. *1. The evident symmetry between $D = \overline{D}$ and $D^{\perp}$ in (2.4) and (2.5) shows that*

$$\overline{D} = (D^{\perp})^{\perp} \tag{2.6}$$

and that the vector $\xi_{\perp}$ is the projection of ξ on $D^{\perp}$.

2. It is also evident that if D is dense in $\mathfrak{H}$, then $D^{\perp} = \{0\}$, and conversely.

One of the corollaries is a criterion for D to be dense and a criterion for a sequence to be complete. We formulate it as a lemma for future reference.

Lemma 2.4. *A subspace D is dense, $\overline{D} = \mathfrak{H}$, iff $\eta \perp D \Longrightarrow \eta = 0$, and a sequence $\{\xi_n\}_1^{\infty}$ is complete, $\overline{L\left(\{\xi_n\}_1^{\infty}\right)} = \mathfrak{H}$, iff $(\eta, \xi_n) = 0,\ \forall n \Longrightarrow \eta = 0$.*

The completeness of an orthonormal basis implies that each vector $\xi \in \mathfrak{H}$ can be expanded with respect to the orthonormal basis, $\xi = \sum_{n=1}^{\infty} a_n e_n$, in the sense that $\lim_{N\to\infty} \sum_{i=1}^{N} a_n e_n = \xi$, where $a_n = (e_n, \xi)$ are the Fourier coefficients with respect to this basis, and Parseval's equality $\|\xi\|^2 = \sum_{n=1}^{\infty} |a_n|^2$ holds.

So, separability implies the possibility of representing any vector as an expansion with respect to an orthonormal basis. In other words, a separable $\mathfrak{H}$ can be considered an infinite orthogonal sum of one-dimensional subspaces spanned by the vectors of the orthonormal basis. It follows that all separable Hilbert spaces are isomorphic.

Any closed subspace $D \subset \mathfrak{H}$ is either a Euclidian space, if it is finite dimensional, or a separable Hilbert space, if it is infinite dimensional (an orthonormal basis in D is provided by orthogonalized nonzero projections $\{e_{n\|}\}$ of an original orthonormal basis $\{e_n\}_1^\infty$ onto D). Any infinite-dimensional closed subspace $D \subset \mathfrak{H}$ is thus isomorphic to the whole of $\mathfrak{H}$ (one of the paradoxes of infinities).

Any s.a. operator with discrete spectrum generates an orthonormal basis in $\mathfrak{H}$ as the set of all its eigenvectors. For example, the sequence $\{e_n\}_1^\infty$ of vectors $e_n = \{\delta_{nm}\}_1^\infty$ with zero components except unity in the mth row is an orthonormal basis in l^2: the orthonormality is evident; the completeness is also clear: $(\xi, e_n) = \overline{x_n} = 0, \forall n$, implies $\xi = 0$ (in particular, this shows once again that l^2 is separable). This orthonormal basis is the set of eigenvectors of the s.a. "particle number" operator $\hat{n}$ (the name is borrowed from QM), $\hat{n}\xi = \{nx_n\}_1^\infty$.

Observables in QM are s.a. operators, and Parseval's equality provides the quantum-mechanical probabilistic interpretation of the Fourier coefficients for the corresponding observables. An s.a. operator with continuous spectrum generates the so-called generalized orthonormal basis.

2.1.3 The Hilbert Space $L^2(a,b)$

Definition 2.5. The Hilbert space $L^2(a,b)$ is the linear space of square-integrable functions on an interval (a,b) of the real axis,

$$L^2(a,b) = \left\{ \psi(x) : \int_a^b \mathrm{d}x \, |\psi(x)|^2 < \infty \right\}.$$

The scalar product in $L^2(a,b)$ is defined by

$$(\psi_1, \psi_2) = \int_a^b \mathrm{d}x \overline{\psi_1(x)} \psi_2(x).$$

It is significant that the integrals are Lebesgue integrals, and strictly speaking, the elements of $L^2(a,b)$ are equivalence classes of functions that are equal almost everywhere.[7]

The correctness of the definition is evident; for a proof of completeness, see, for example, [9].

The endpoints a and b of an interval can be infinities, $a = -\infty$ and/or $b = +\infty$, and in particular, the case of $a = -\infty$, $b = \infty$ corresponds to the whole real

[7]When speaking about some function belonging to $L^2(a,b)$ and possessing some additional specific properties like absolute continuity, we actually mean the representative of the corresponding equivalence class.

axis $\mathbb{R}$, while the case of $a = 0$, $b = \infty$ corresponds to the semiaxis $\mathbb{R}_+$. By convention, see Chap. 1, the finite endpoints of an interval are considered to belong to the interval, so that by a finite interval is meant a closed interval $[a, b]$ and by a positive semiaxis is meant $\mathbb{R}_+$. This is simply a matter of convenience, because the measure of the endpoints is equal to zero, but under this convention, the boundary values of functions $\psi(x)$ at finite endpoints, for example $\psi(a)$, have an obvious sense. We also adopt the following convention on terminology relating to functions defined on an interval (a, b) with at least one finite endpoint. The term "in an interval" concerns all the interior points of the interval, i.e., the open interval (a, b), while the term "on an interval" concerns all the points of the interval including its finite endpoints, i.e. the whole interval.

It is useful to note that every function $\psi(x)$ belonging to $L^2(a, b)$ is locally integrable on the interval,[8] which follows from the Cauchy–Schwarz inequality, and therefore allows the representation $\psi(x) = \Psi'(x)$, where $\Psi(x) = \int_c^x \mathrm{d}y\,\psi(y)$, $c \in (a, b)$, is a *function absolutely continuous on the interval* (a, b) (*a.c. function* in what follows). We recall that one of the equivalent definitions of an a.c. function reads as follows: a function $\Psi(x)$ defined on an interval (a, b) is said to be a.c. in the interval if it can be represented as

$$\Psi(x) = \int_{x_0}^{x} \mathrm{d}y\,\psi(y) + \Psi(x_0), \quad a < x_0 < b,$$

in which case $\psi(x) = \Psi'(x)$ almost everywhere. In other words, an a.c. function is differentiable almost everywhere and is restored in the interval by integrating its derivative. If the left endpoint a is finite and the integral on the right-hand side exists for $x = a$ (which is the case if $\psi(x)$ is square-integrable on (a, b)), then $\Psi(x)$ is continuous up to the left endpoint and has a boundary value $\Psi(a)$. The same can be said about the right endpoint b. Absolutely continuous functions can be integrated by parts in the usual way.

If $(a, b) \subset (c, d)$, the Hilbert space $L^2(a, b)$ can be considered a closed subspace in $L^2(c, d)$, $L^2(a, b) \subset L^2(c, d)$, and any $L^2(a, b)$ can be considered a closed subspace in $L^2(\mathbb{R})$.

Hilbert spaces $L^2(a, b)$ are of paramount importance for QM, and they are extensively exploited in the present book.

Let $\mathcal{D}(a, b)$ be a *linear complex space of smooth compactly supported functions on the interval*[9] (a, b):

$$\mathcal{D}(a, b) = \{\varphi(x) : \varphi(x) \in \mathbb{C}^\infty(a, b),\ \operatorname{supp}\varphi \subseteq [\alpha, \beta] \subset (a, b)\},$$

[8] By local integrability on an interval (a, b), we mean the (absolute) integrability on any finite interval $[\alpha, \beta]$ belonging to (a, b), $a \le \alpha < \beta \le b$, where the equality signs are meaningful for finite endpoints; by local integrability in an interval (a, b), we mean the integrability on any finite interval $[\alpha, \beta]$ within (a, b), $a < \alpha < \beta < b$.

[9] In the Russian mathematical literature, a smooth compactly supported function is known as a "finitnaya" function.

where $\mathbb{C}^{\infty}(a,b)$ is the *linear space of smooth, or infinitely differentiable, functions on the interval* (a,b); as usual, we let $\operatorname{supp}\varphi$ denote the support of φ, the closure of the set of points x where $\varphi(x) \neq 0$; α and β are generally different for different φ. The condition on $\operatorname{supp}\varphi$ is that it be contained entirely inside the interval (a,b), and each function belonging to $\mathcal{D}(a,b)$ vanishes in some neighborhood of the endpoints a and b of the interval. It is evident that $\mathcal{D}(a,b) \subset L^2(a,b)$.

We define some other useful spaces of functions that appear in our considerations below.

$D(a,b)$ is the *linear space of arbitrary functions on the interval* (a,b) *with compact support*:

$$\varphi(x) \in D(a,b) \Longrightarrow \operatorname{supp}\varphi \subseteq [\alpha,\beta] \subset (a,b);$$

$D_r(a,b)$ is the *linear space of arbitrary functions on the interval* (a,b) *with support bounded from the right* :

$$\varphi(x) \in D_r(a,b) \Longrightarrow \operatorname{supp}\varphi \subseteq [a,\beta]\,,\ \beta < b;$$

$D_l(a,b)$ is the *linear space of arbitrary functions on the interval* (a,b) *with support bounded from the left*:

$$\varphi(x) \in D_l(a,b) \Longrightarrow \operatorname{supp}\varphi \subseteq [\alpha,b]\,,\ \alpha > a;$$

$\mathcal{D}_R(a,b)$ is the *linear space of real smooth compactly supported functions on the interval* (a,b):

$$\varphi(x) \in \mathcal{D}_R(a,b) \Longrightarrow \varphi(x) = \overline{\varphi(x)} \in \mathcal{D}(a,b),$$

$\mathcal{D}_R(a,b)$ is a real subspace of $\mathcal{D}(a,b)$.

Theorem 2.6. *The subspace* $\mathcal{D}(a,b)$ *is dense in* $L^2(a,b)$, $\overline{\mathcal{D}(a,b)} = L^2(a,b)$.

A proof of this theorem is based on two lemmas in the theory of real functions.

Lemma 2.7. *Let* $\psi(x)$ *be a continuous real function on* (a,b). *Then the condition*

$$\int_a^b \mathrm{d}x\,\psi(x)\,\varphi(x) = 0\,,\ \forall\varphi(x) \in \mathcal{D}_R(a,b),$$

implies that $\psi(x) = 0$.

Proof. Assume the contrary. Let $x_0 \in (a,b)$ be an inner point of (a,b), and let $\psi(x_0) \neq 0$, for example, $\psi(x_0) > 0$ (the arguments for the case of $\psi(x_0) < 0$ are the same). Then there exists a closed interval $[x_0 - \varepsilon_0, x_0 + \varepsilon_0] \subset (a,b)$, $\varepsilon_0 > 0$, where $\psi(x_0) > 0$.

On the other hand, there exists a function $\varphi_\varepsilon(x) \in \mathcal{D}_R(a,b)$ such that $\operatorname{supp}\varphi_\varepsilon = [x_0 - \varepsilon_0, x_0 + \varepsilon_0]$ and $\varphi(x) > 0$ for $x \in (x_0 - \varepsilon_0, x_0 + \varepsilon_0)$, and we have

$$\int_a^b \mathrm{d}x \psi(x) \varphi_\varepsilon(x) = \int_{x_0-\varepsilon_0}^{x_0+\varepsilon_0} \mathrm{d}x \psi(x) \varphi_\varepsilon(x) > 0,$$

which contradicts the condition and thus proves the lemma. □

Lemma 2.8. *Let $\psi(x)$ be a continuous real function on (a,b). Then the condition*

$$\int_a^b \mathrm{d}x \psi(x) \phi'(x) = 0\,, \ \forall \phi(x) \in \mathcal{D}_R(a,b)\,, \tag{2.7}$$

implies that $\psi(x) = \mathrm{c} = \mathrm{const}$.

A proof of Lemma 2.8 is based on the following simple lemma and its corollary.

Lemma 2.9. *Let $\chi(x) \in \mathcal{D}_R(a,b)$. Then $\chi(x) = \varphi'(x)\,,\ \varphi(x) \in \mathcal{D}_R(a,b)$ iff $\int_a^b \mathrm{d}x \chi(x) = 0$. In addition, if $\operatorname{supp}\chi \subseteq [\alpha,\beta] \subset (a,b)$, then $\operatorname{supp}\varphi \subseteq [\alpha,\beta]$ as well.*

Proof. Necessity. Let $\chi(x) \in \mathcal{D}_R(a,b)$ and let $\chi(x) = \varphi'(x)$, $\varphi(x) \in \mathcal{D}_R(a,b)$. It follows from the definition of $\mathcal{D}_R(a,b)$ that

$$\int_a^b \mathrm{d}x \chi(x) = \int_a^b \mathrm{d}x \varphi'(x) = \varphi(x)|_a^b = 0$$

because $\varphi(x)$ vanishes outside of its support that is strictly inside of (a,b). It is also easy to see that if $\operatorname{supp}\chi \subseteq [\alpha,\beta] \subset (a,b)$, then $\varphi(x) = \int_a^x \mathrm{d}y \chi(y)$ must be zero outside of $[\alpha,\beta]$ (the corresponding reasoning is similar to that below in proving sufficiency).

Sufficiency. Let $\chi(x) \in \mathcal{D}_R(a,b)$, let $\operatorname{supp}\chi \subseteq [\alpha,\beta] \subset (a,b)$, and let

$$\int_a^b \mathrm{d}x \chi(x) = \int_\alpha^\beta \mathrm{d}x \chi(x) = 0. \tag{2.8}$$

We consider the function $\varphi(x)$ given by

$$\varphi(x) = \int_a^x \mathrm{d}y \chi(y) = \int_\alpha^x \mathrm{d}y \chi(y)\,.$$

It is evident that $\varphi(x) \in \mathbb{C}^\infty(a,b)$ and $\chi(x) = \varphi'(x)$. Because $\chi(x) = 0$, $x < \alpha$, we have $\varphi(x) = 0$ for $x < \alpha$, while for $x > \beta$, we have

$$\varphi(x) = \int_\alpha^x \mathrm{d}y \chi(y) = \int_\alpha^\beta \mathrm{d}y \chi(y) = 0$$

because of $\chi(x) = 0$, $x > \beta$, and condition (2.8). This means that $\operatorname{supp}\varphi \subseteq [\alpha,\beta]$, which proves the lemma. □

Corollary 2.10. *Any function* $\varphi(x) \in \mathcal{D}_R(a,b)$ *allows the representation*

$$\varphi(x) = c(\varphi)\varphi_0(x) + \phi'(x), \;\; c(\varphi) = \int_a^b \mathrm{d}x\varphi(x)\,, \tag{2.9}$$

with some $\varphi_0(x) \in \mathcal{D}_R(a,b)$ *such that* $\int_a^b \mathrm{d}x\varphi_0(x) = 1$ *and some* $\phi(x) \in \mathcal{D}_R(a,b)$.

A function $\varphi_0(x)$ with the indicated properties does exist: it is sufficient to take any function $\varphi(x) \in \mathcal{D}_R(a,b)$ with $\int_a^b \mathrm{d}x\varphi(x) \neq 0$. Then the function

$$\varphi_0(x) = \left[\int_a^b \mathrm{d}y\varphi(y)\right]^{-1} \varphi(x)$$

is the required one. We then consider the function $\chi(x) = \varphi(x) - c(\varphi)\varphi_0(x)$ with the evident properties: $\chi(x) \in \mathcal{D}_R(a,b)$ and

$$\int_a^b \mathrm{d}x\,\chi(x) = \int_a^b \mathrm{d}x\,[\varphi(x) - c(\varphi)\varphi_0(x)] = c(\varphi) - c(\varphi)\int_a^b \mathrm{d}x\varphi_0(x) = 0\,.$$

It follows from Lemma 2.9 that $\chi(x) = \phi'(x)$, $\phi(x) \in \mathcal{D}_R(a,b)$, which gives representation (2.9).

Proof of Lemma 2.8. We take any $\varphi \in \mathcal{D}_R(a,b)$. According to representation (2.9), we have $\varphi(x) - c(\varphi)\varphi_0(x) = \phi'(x)$, $\phi \in \mathcal{D}_R(a,b)$. With this $\phi'(x)$, the left-hand side in (2.7) becomes

$$\int_a^b \mathrm{d}x\psi(x)\,\phi'(x) = \int_a^b \mathrm{d}x\,[\psi(x) - \mathrm{c}]\,\varphi(x)\,,$$

where $\mathrm{c} = \int_a^b \mathrm{d}y\psi(y)\,\varphi_0(y) = \text{const}$, and condition (2.7) becomes

$$\int_a^b \mathrm{d}x\,[\psi(x) - \mathrm{c}]\,\varphi(x) = 0\,, \;\; \forall\varphi(x) \in \mathcal{D}_R(a,b)\,.$$

By Lemma 2.7, it follows that $\psi(x) = \mathrm{c}$, which completes the proof of Lemma 2.8. □

We can now return to the theorem.

Proof of Theorem 2.6. By virtue of Lemma 2.4 it is sufficient to prove that

$$\int_a^b \mathrm{d}x\overline{\psi(x)}\varphi(x) = 0\,, \;\; \psi \in L^2(a,b)\;, \;\; \forall\varphi \in \mathcal{D}(a,b)\,,$$

implies that $\psi(x) = 0$ (almost everywhere). It is easy to see that this assertion is equivalent to a similar assertion for real-valued functions $\psi(x)$ and $\varphi(x)$. We therefore assume that $\psi(x)$ and $\varphi(x)$ are real-valued functions and prove that the condition

$$\int_a^b \mathrm{d}x\, \psi(x)\, \varphi(x) = 0\,,\ \ \forall\varphi(x) \in \mathcal{D}_R(a,b)\,, \tag{2.10}$$

implies that $\psi(x) = 0$ (almost everywhere).

For this purpose, we use the above-cited representation $\psi(x) = \Psi'(x)$ with $\Psi(x) = \int_c^x \mathrm{d}y\, \psi(y)$, $c \in (a,b)$, for a locally integrable function $\psi(x)$. Substituting this representation into the left-hand side in (2.10), integrating by parts, and taking into account that $\varphi(x)$ vanishes near both endpoints a and b, we convert condition (2.10) into the condition

$$\int_a^b \mathrm{d}x \Psi(x)\, \varphi'(x) = 0\,,\ \ \forall\varphi(x) \in \mathcal{D}_R(a,b)$$

for a continuous function $\Psi(x)$. It then follows from Lemma 2.8 that $\Psi(x) = c =$ const, and therefore, $\psi(x) = 0$ almost everywhere. The theorem is proved. □

Remark 2.11. We note that in fact, the proof of the theorem is reduced to a proof of the extension of Lemma 2.7 to locally integrable functions.

Lemma 2.8 also allows a similar extension.

Lemma 2.12 (Du Bois–Reymond lemma). *Let $\psi(x)$ be a locally integrable real function on (a,b). Then the condition*

$$\int_a^b \mathrm{d}x\, \psi(x)\, \phi'(x) = 0\,,\ \ \forall\phi(x) \in \mathcal{D}_R(a,b)\,,$$

implies that $\psi(x) = \mathrm{c} = \mathrm{const}$ almost everywhere.

The proof of this lemma is similar to that of Lemma 2.8: we take any $\varphi(x) \in \mathcal{D}_R(a,b)$, use representation (2.9), substitute the respective $\phi'(x) = \varphi(x) - c(\varphi)\varphi_0(x)$ into the defining integral of the condition of the lemma, and reduce this condition to the equivalent condition

$$\int_a^b \mathrm{d}x\, (\psi(x) - \mathrm{c})\, \varphi(x) = 0\,,\ \ \forall\varphi(x) \in \mathcal{D}_R(a,b)\,,$$

where $\mathrm{c} = \int_a^b \mathrm{d}y\, \psi(y)\, \varphi_0(y) = \mathrm{const}$. It then follows from the extended version of Lemma 2.7 that $\psi(x) = \mathrm{c}$ almost everywhere.

Different sets of functions are known as orthonormal bases in the Hilbert space $L^2(a,b)$; of course, they are different for different intervals. We cite only the best-known ones.

The Hermite functions

$$H_n(x) = \left(\sqrt{\pi}2^n n!\right)^{-\frac{1}{2}} e^{\frac{x^2}{2}} d_x^n e^{-x^2},\ n \in \mathbb{Z}_+,$$

form an orthonormal basis in $L^2(\mathbb{R})$. A proof can be found in [9]. It follows that the Hilbert space $L^2(\mathbb{R})$ is separable, and therefore, every Hilbert space $L^2(a,b)$ is also separable as a closed subspace in $L^2(\mathbb{R})$. The Hermite functions are the eigenfunctions of the s.a. QM oscillator Hamiltonian $\hat{H} = -d_x^2 + x^2$. The isomorphism between l^2 and $L^2(\mathbb{R})$ is realized by the mapping $e_n \leftrightarrows H_n(x)$ extended by linearity. One of the orthonormal bases in $L^2(\mathbb{R}_+)$ is given by the Laguerre functions, while one of the orthonormal bases in $L^2(-1,1)$ is given by the Legendre polynomials.[10]

In conclusion, we consider a relation between the behavior of functions at infinity and their square-integrability at infinity. This remark concerns functions belonging to Hilbert spaces $L^2(a,b)$ where the interval (a,b) is infinite, i.e., $a = -\infty$ or/and $b = \infty$. The notion of square-integrability at infinity is an extension of the notion of local square-integrability to a point at infinity. We call a function $\psi(x)$ square-integrable at ∞ (plus infinity) if $\int_c^\infty |\psi(x)|^2 < \infty$ for some finite c, i.e., $\psi(x) \in L^2(c,\infty)$ for $x \geq c > -\infty$. The square-integrability at $-\infty$ (minus infinity) is defined similarly. An assertion is rather common in the physics literature that the square-integrability of a wave function at plus or minus infinity implies that the function vanishes at the respective infinity, for example, if $\psi(x) \in L^2(\mathbb{R})$, then $\psi(x) \to 0$ as $x \to \pm\infty$. This assertion is wrong: it is easy to construct a function that belongs to $L^2(\mathbb{R})$ and takes arbitrarily large values at arbitrarily large $|x|$. An example is given by

$$\psi(x) = \begin{cases} n,\ n - n^{-4} < x < n,\ |n| \in \mathbb{N}, \\ 0 \text{ elsewhere.} \end{cases}$$

But if a function is a.c. at infinity and is square-integrable at infinity together with its first derivative, then it does vanish at infinity.

Lemma 2.13. *Let a function $\psi(x)$ be a.c. for $x \geq c$ ($x \leq c$), $|c| < \infty$, and let $\psi, \psi' \in L^2(c,\infty)$ ($L^2(-\infty,c)$). Then $\psi(x) \to 0$ as $x \to \infty$ ($-\infty$).*

Proof. We give a proof for the case (c,∞); a proof for the case $(-\infty,c)$ is completely similar. We consider the identity

$$\left|\psi^2(x)\right| = \int_c^x dy \left(\overline{\psi(y)}\psi'(y) + \overline{\psi'(y)}\psi(y)\right) + \left|\psi^2(c)\right|.$$

[10] A subtlety is that the set of powers of x, $\{x^k\}_0^\infty$, is a complete sequence in $L^2(-1,1)$, but it does not form a basis [9].

Because $\psi, \psi' \in L^2(c,\infty)$, the integral on the right-hand side has a finite limit as $x \to \infty$. It follows that $|\psi(x)|$ has a finite limit as $x \to \infty$. This limit must be zero because of the square-integrability of $\psi(x)$ at infinity, which proves the lemma. □

The next lemma can be also useful.

Lemma 2.14. *Let $\psi(x)$ and $\psi'(x)$ be a.c. for $x \geq c$ ($x \leq c$), $|c| < \infty$, and let $\psi, \psi'' \in L^2(c,\infty)(L^2(-\infty,c))$. Then $\psi' \in L^2(c,\infty)$ $(L^2(-\infty,c))$, and $\psi(x), \psi'(x) \to 0$ as $x \to \infty$ $(-\infty)$.*

Proof. We give a proof for the case (c,∞); a proof for the case $(-\infty,c)$ is completely similar. We consider the identity

$$d_x |\psi(x)|^2 = 2\int_c^x \mathrm{d}y \left|\psi'(y)\right|^2 + \int_c^x \mathrm{d}y \left[\overline{\psi(y)}\psi''(y) + \overline{\psi''(y)}\psi(y)\right] + d_x |\psi(x)|^2\Big|_{x=c}.$$

Because $\psi, \psi'' \in L^2(c,\infty)$, the second integral on the right-hand side has a finite limit as $x \to \infty$. It follows that if $\int_c^x \mathrm{d}y\, |\psi'(y)|^2 \to \infty$ as $x \to \infty$, then $d_x |\psi(x)|^2 \to \infty$ as $x \to \infty$ as well. But if this is the case, then $|\psi(x)|^2 \to \infty$ as $x \to \infty$, which contradicts the square-integrability of ψ at infinity. We thus obtain that there must be $\int_c^\infty \mathrm{d}y\, |\psi'(y)|^2 < \infty$, which proves the first assertion of the lemma. The second assertion then immediately follows from Lemma 2.13. □

In QM, the Hilbert space $L^2(a,b)$ is the space of states for a particle moving on an interval (a,b) of the real axis. For a particle moving in a multidimensional space or for many-particle systems, appropriate spaces of states are Hilbert spaces $L^2(\mathbb{R}^n)$, $n = 2,3,\ldots$. For example, the space of states for n particles, $n = 2,3,\ldots$, moving in the three-dimensional space $\mathbb{R}^3$ is the Hilbert space $L^2(\mathbb{R}^{3n})$. A definition of a Hilbert space $L^2(\mathbb{R}^n)$ is a copy of the above definition of the Hilbert space $L^2(a,b)$ with the evident substitution of integrals over (a,b) for the respective integrals over $\mathbb{R}^n$. For a system of n particles moving in a volume $V \subset \mathbb{R}^3$, the space of states is reduced to $L^2(V^n)$.

Physical systems with varying or nonconserving number of particles are described in terms of orthogonal direct sums of $L^2(\mathbb{R}^n)$ with different n. An example from the many-body theory and quantum field theory is the so-called Fock space F:

$$F = \sum_{n=0}^{\infty}{}^{\oplus} L^2\left(\mathbb{R}^{3n}\right), \quad L^2\left(\mathbb{R}^0\right) = \mathbb{C}.$$

Vectors of the Fock space F are Fock columns whose first component is a complex number c, while other components are functions of increasing number of space variables $\psi_1(\mathbf{r}_1), \psi_2(\mathbf{r}_1,\mathbf{r}_2), \ldots, \psi_n(\mathbf{r}_1,\ldots,\mathbf{r}_n), \ldots$, where $\mathbf{r} \in \mathbb{R}^3$ and $\psi_n(\mathbf{r}_1,\ldots,\mathbf{r}_n) \in L^2\left(\mathbb{R}^{3n}\right)$.

For identical bosons or fermions, these functions are respectively symmetric or antisymmetric with respect to transpositions of arguments.

We now turn to functions in Hilbert spaces. We restrict ourselves to linear functions: linear functionals and linear operators.

2.2 Linear Functionals

Definition 2.15. A *linear functional* $\varPhi$ in $\mathfrak{H}$ with a domain of definition, or simply domain, $D_\varPhi \subseteq \mathfrak{H}$ is a linear mapping $\varPhi : D_\varPhi \longmapsto \mathbb{C}$; this means that $D_\varPhi$ is a subspace and that any vector $\xi \in D_\varPhi$ is assigned a complex number $z = \varPhi(\xi)$, or $\xi \overset{\varPhi}{\longmapsto} \varPhi(\xi) \in \mathbb{C}$, $\forall \xi \in D_\varPhi$, so that

$$\varPhi\left(a_1\xi_1 + a_2\xi_2\right) = a_1\varPhi\left(\xi_1\right) + a_2\varPhi\left(\xi_2\right), \quad \forall \xi_1, \xi_2 \in D_\varPhi, \quad \forall a_1, a_2 \in \mathbb{C}.$$

We only cite (as a rule, without proof) some necessary facts and notions from the theory of linear functionals that we shall need later when expounding the theory of linear operators in $\mathfrak{H}$. The details of the theory of linear functionals can be found, for example, in [9].

In connection with the topology in $\mathfrak{H}$ and the usual topology in $\mathbb{C}$, the natural notions of boundedness and continuity are introduced for linear functionals.

A linear functional $\varPhi$ is called bounded if there exists a finite nonnegative number K such that

$$\left|\varPhi\left(\xi\right)\right| \leq K \left\|\xi\right\| , \ \forall \xi \in D_\varPhi .$$

The norm $\|\varPhi\|$ of a functional $\varPhi$ is the infimum of such K's. It is evident that $\left|\varPhi\left(\xi\right)\right| \leq \|\varPhi\| \, \|\xi\|$ and $\varPhi$ is bounded iff its norm is finite.

A linear functional $\varPhi$ is called continuous if

$$\xi \,, \ \xi_0 \in D_\varPhi \,, \ \xi \longrightarrow \xi_0 \Longrightarrow \varPhi\left(\xi\right) \longrightarrow \varPhi\left(\xi_0\right), \ \forall \xi_0 \in D_\varPhi \,.$$

It is evident that a linear functional $\varPhi$ is continuous iff it is continuous at the origin,

$$\xi \in D_\varPhi \,, \ \xi \longrightarrow 0 \Longrightarrow \varPhi\left(\xi\right) \longrightarrow 0 \,.$$

The notions of boundedness and continuity are equivalent for linear functionals: a linear functional is continuous iff it is bounded. We note only that sufficiency is evident from the inequality $\left|\varPhi\left(\xi\right)\right| \leq \|\varPhi\| \, \|\xi\|$.

A bounded linear functional with domain $D_\varPhi \neq \mathfrak{H}$ can be extended to the whole of $\mathfrak{H}$ without changing its norm: it is first extended to the closure $\overline{D_\varPhi}$ of its domain by continuity and is then defined by zero on the orthogonal complement

$\overline{D_\Phi}^{\perp}$ of D_Φ. Therefore, bounded linear functionals can be considered as defined everywhere without loss of generality.[11]

The kernel of a linear functional Φ, denoted by $\ker\Phi$, is the set of all vectors ξ such that $\Phi(\xi) = 0$, $\ker\Phi = \{\xi : \Phi(\xi) = 0\}$. It is evident that the kernel of a linear functional is a subspace, and if the functional is bounded and defined everywhere, its kernel is a closed subspace, $\ker\Phi = \overline{\ker\Phi}$.

Theorem 2.16 (Riesz theorem). *Any bounded linear functional defined everywhere has the form* $\Phi(\xi) = (\eta, \xi)$ *with some* $\eta \in \mathfrak{H}$*; its norm is given by* $\|\Phi\| = \|\eta\|$*, and its kernel is given by* $\ker\Phi = \{\xi : \xi \perp \eta\}$.

Proof. The proof is so simple and instructive that we reproduce it here. For $\Phi = 0$, the assertion is evident: $\eta = 0$. Let $\Phi \neq 0$. Because $\ker\Phi$ is a closed subspace, the decomposition

$$\mathfrak{H} = \ker\Phi \oplus (\ker\Phi)^{\perp}$$

holds. Let $\zeta \in (\ker\Phi)^{\perp}$, $\Phi(\zeta) \neq 0$. For any vector ξ, the vector $\Phi(\zeta)\,\xi - \Phi(\xi)\,\zeta$ evidently belongs to $\ker\Phi$ and is therefore orthogonal to ζ, i.e., $\Phi(\zeta)(\zeta, \xi) - \Phi(\xi)\|\zeta\|^2 = 0$. It follows that

$$\Phi(\xi) = \Phi(\zeta^{\mathrm{n}})(\zeta^{\mathrm{n}}, \xi) = (\eta, \xi), \ \eta = \overline{\Phi(\zeta^{\mathrm{n}})}\zeta^{\mathrm{n}}, \ \zeta^{\mathrm{n}} = \zeta / \|\zeta\|.$$

It is evident that η is defined uniquely (and therefore, $(\ker\Phi)^{\perp}$ is a one-dimensional subspace): the relation $(\eta', \xi) = (\eta, \xi)$, $\forall\xi \in \mathfrak{H}$, implies $(\eta' - \eta, \xi) = 0$, $\forall\xi \in \mathfrak{H}$, or $(\eta' - \eta) \perp \mathfrak{H}$, which in turn implies that $\eta' - \eta = 0$, or $\eta' = \eta$. The equality $\|\Phi\| = \|\eta\|$ follows from the Cauchy–Schwarz inequality, while the formula for the kernel of Φ is evident. □

Bounded linear functionals naturally form a linear space that is called a dual space: $\Phi = a_1\Phi_1 + a_2\Phi_2$ is defined by

$$(a_1\Phi_1 + a_2\Phi_2)(\xi) = a_1\Phi_1(\xi) + a_2\Phi_2(\xi).$$

The Riesz theorem, Theorem 2.16, shows that there exists an anti-isomorphism between $\mathfrak{H}$ and its dual space.

The notion of a linear functional allows introducing the so-called *weak topology* in $\mathfrak{H}$, in particular, weak boundedness and weak convergence. As for the conventional topology, we call it the *strong topology* and speak about *strong boundedness* and *strong convergence*.

A set $M \subset \mathfrak{H}$ is weakly bounded if the values of any functional on M are uniformly bounded, i.e., $|(\eta, \xi)| < C(\eta)$, $\forall\xi \in M$, $\forall\eta \in \mathfrak{H}$.

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[11] Encountered unbounded linear functionals cannot be defined in the whole Hilbert space: an unbounded linear functional defined everywhere is equal to zero almost everywhere. The requirement of boundedness is often included in the definition of a linear functional.

A sequence $\{\xi_k\}_1^\infty$ is called weakly convergent to a vector ξ, which is written $\mathrm{wlim}_{k\to\infty}\xi_k = \xi$, if

$$\lim_{k\to\infty} (\eta\,,\xi_k) = (\eta, \xi)\,,\ \ \forall\eta \in \mathfrak{H}.$$

In a finite-dimensional Euclidean space, the strong and weak topologies are equivalent. In an infinite-dimensional Hilbert space, these topologies are not equivalent; indeed, the strong topology is stronger than the weak topology, i.e., strong convergence implies weak convergence:

$$\lim_{k\to\infty} \xi_k = \xi \Longrightarrow \xi_k \xrightarrow{w} \xi,\ k \to \infty,\ \text{or}\ \xi = \mathrm{wlim}_{k\to\infty}\xi_k\,.$$

A proof follows from the Cauchy–Schwarz inequality. But the converse generally does not hold. A counterexample is given by an orthonormal basis $\{e_k\}_1^\infty$: $\lim_{k\to\infty} (\eta, e_k) = 0, \forall\eta \in \mathfrak{H}$, because of the Parseval equality, i.e., $\mathrm{wlim}_{k\to\infty}e_k = 0$, whereas $\{e_k\}_1^\infty$ is not a Cauchy sequence, $\|e_k - e_l\| = \sqrt{2}$, $\forall k \neq l$.

As for the relation between strong boundedness and weak boundedness, it is clear that strong boundedness implies weak boundedness because of the Cauchy–Schwarz inequality. It appears that the converse also holds.

Theorem 2.17. *The weak boundedness of a set $M \subset \mathfrak{H}$ is equivalent to its strong boundedness.*

An elegant proof of this theorem can be found in [87].

2.3 Linear Operators

2.3.1 Definitions and General Remarks

The notion of linear operator in a Hilbert space is a direct generalization of the notion of linear transformation in a finite-dimensional Euclidean space. But in Euclidean spaces, linear transformations can be and are usually defined in the whole space, while in an infinite-dimensional Hilbert space, this is generally not the case, and the notion of domain of a linear operator takes on great importance. The same transformation ("rule of acting") applied to different domains determines different operators with sometimes crucially different properties. This is particularly true for the unbounded operators, which are absent in the finite-dimensional case.

Definition 2.18. A *linear operator* $\hat{f}$ with a *domain of definition*, or simply domain, $D_f \subseteq \mathfrak{H}$ is a linear mapping of D_f to $\mathfrak{H}$, $\hat{f}\ :\ D_f \longrightarrow \mathfrak{H}$; this means that D_f is a subspace and that any vector $\xi \in D_f$ is assigned some vector $\eta = \hat{f}\xi$, or

$$\xi \xrightarrow{f} \hat{f}\xi \in \mathfrak{H},\ \forall\xi \in D_f$$

(this is the "rule of acting"), so that

$$\hat{f}(a_1\xi_1 + a_2\xi_2) = a_1\,\hat{f}\xi_1 + a_2\,\hat{f}\xi_2\,,\ \forall\xi_1,\xi_2 \in D_f,\ \forall a_1,a_2 \in \mathbb{C}\,.$$

We emphasize that in contrast to linear functionals, the continuity (or boundedness) of linear operators is not required. Many QM observables are discontinuous (unbounded).

A vector $\eta = \hat{f}\xi$ is called the image of a vector ξ, and ξ is called the preimage of η. The set of all images, sometimes denoted by $\hat{f}D_f$, is called the *range of the operator* $\hat{f}$, and is denoted by R_f,

$$R_f = \hat{f}D_f = \{\eta : \eta = \hat{f}\xi,\ \forall\xi \in D_f\}\,.$$

If $D_f = \mathfrak{H}$, the operator $\hat{f}$ is said to be defined everywhere; it is typical for bounded (or continuous) operators.

In general, D_f is not a closed subspace, $D_f \neq \overline{D_f}$; it is typical for unbounded (or discontinuous) operators, and is a specific feature of an infinite-dimensional $\mathfrak{H}$.

If $\overline{D_f} = \mathfrak{H}$, the operator $\hat{f}$ is called a *densely defined operator*; it is typical for QM observables. In general, $R_f \neq \overline{R_f}$, and even $\overline{R_f} \neq \mathfrak{H}$.

A number λ is called an eigenvalue of an operator $\hat{f}$ if there exists a nonzero vector $\xi_\lambda \in D_f$ such that $\hat{f}\xi_\lambda = \lambda\xi_\lambda$; the vector ξ_λ is called an eigenvector of $\hat{f}$ corresponding to the eigenvalue λ. The set of all eigenvectors corresponding to an eigenvalue λ supplemented with the zero vector is called the eigenspace of $\hat{f}$ corresponding to the eigenvalue λ; it is evident that an eigenspace is a subspace belonging to D_f. The dimension of an eigenspace corresponding to an eigenvalue λ is called the multiplicity of the eigenvalue. If $\mathfrak{H}$ is a space of functions like $L^2(a,b)$, the eigenvectors are also called eigenfunctions.

We note that there is a stable distinction between the physical and mathematical terminologies at this point. As an illustration, we consider the operator $\hat{p} = -i\hbar d_x$ in $L^2(\mathbb{R})$ that is the momentum operator for a particle moving along the real axis (its domain is defined below). In physics textbooks, the function $\psi_p(x) = \exp(\mathrm{i}px/\hbar)$ satisfying the differential equation $-i\hbar\psi_p'(x) = p\psi_p(x)$ is called the eigenfunction of the momentum corresponding to the eigenvalue p. But the function $\exp(\mathrm{i}px/\hbar)$ does not belong to the Hilbert space $L^2(\mathbb{R})$ because it is not square-integrable on the whole axis (more specifically, not square-integrable at infinity). Therefore, from the standpoint of the adopted definition, $\exp(\mathrm{i}px/\hbar)$ is not an eigenfunction of $\hat{p}$, and p is not its eigenvalue; this function is the so-called generalized eigenfunction of $\hat{p}$, while p is a point of the spectrum of $\hat{p}$ (see below).

Now we list some useful definitions:

(a) We call the number $\left(\xi\,,\hat{f}\xi\right)^{-1}$, $\xi \in D_f$, the *mean of the operator* $\hat{f}$ in the state ξ (the last term is borrowed from QM).

(b) We call an operator $\hat{f}$ nonnegative, written $\hat{f} \geq 0$, if $(\xi, \hat{f}\xi) \geq 0$, $\forall\xi \in D_f$, i.e., if all of its means are nonnegative. We call an operator $\hat{f}$ positive, written

$\hat{f} > 0$ if $(\xi, \hat{f}\xi) > 0$, $\forall \xi \in D_f$, $\xi \neq 0$, i.e., if all of its means for nonzero states are positive. We call an operator $\hat{f}$ nonpositive, written $\hat{f} \leq 0$, or negative, written $\hat{f} < 0$, if the operator $-\hat{f}$ is respectively nonnegative or positive. The inequality $\hat{f}_1 \geq \hat{f}_2$, or $\hat{f}_2 \leq \hat{f}_1$, implies that $D_{f_1} = D_{f_2}$ and means that $\hat{f}_1 - \hat{f}_2 \geq 0$, or $\hat{f}_2 - \hat{f}_1 \leq 0$.

(c) We call an operator $\hat{f}$ bounded from below if $\left(\xi, \hat{f}\xi\right) \geq \gamma\,(\xi, \xi)$, $\forall \xi \in D_f$.

(d) We call an operator $\hat{f}$ bounded from above if $\left(\xi, \hat{f}\xi\right) \leq \gamma\,(\xi, \xi)$, $\forall \xi \in D_f$. Clearly, the constants γ in (c) and (d) are real, $\gamma = \overline{\gamma}$.

2.3.2 Graphs

We now present an equivalent definition of a linear operator in $\mathfrak{H}$ in terms of graphs (this is true for any functions; recall graphs of school functions).

We call a set $G = \{(\xi / \eta)\} \subset \mathbb{H} = \mathfrak{H} \oplus \mathfrak{H}$ a *graph* if its abscissas ξ uniquely determine its ordinates η, i.e.,

$$\left.\begin{array}{l}\{(\xi / \eta)\} \in \mathbb{G} \\ \{(\xi / \zeta)\} \in \mathbb{G}\end{array}\right\} \Longrightarrow \eta = \zeta\,.$$

An equivalent definition of a linear operator in $\mathfrak{H}$ is then as follows:

A linear operator $\hat{f}$ in a Hilbert space $\mathfrak{H}$ is a triple

$$\hat{f} = \mathfrak{H},\ \mathfrak{H},\ \mathbb{G}_f = \left\{\left(\xi / \hat{f}\,\xi\right)\right\} \subset \mathbb{H},$$

where the graph $\mathbb{G}_f$ is a subspace in $\mathbb{H}$, i.e.,

$$\left(\xi_1 / \hat{f}\xi_1\right), \left(\xi_2 / \hat{f}\xi_2\right) \in \mathbb{G}_f \Longrightarrow a_1\left(\xi_1 / \hat{f}\xi_1\right) + a_2\left(\xi_2 / \hat{f}\xi_2\right)$$
$$= \left(a_1\xi_1 + a_2\xi_2 / a_1\,\hat{f}\xi_{1+}a_2\,\hat{f}\xi_2\right) \in \mathbb{G}_f\,.$$

The set of all abscissas of $\mathbb{G}_f$ is the domain D_f of the operator $\hat{f}$, $D_f = \{\xi : (\xi / \hat{f}\xi) \in \mathbb{G}_f\}$; the set of all ordinates of $\mathbb{G}_f$, is the range R_f of the operator $\hat{f}$, $R_f = \{\eta : (\xi / \eta = \hat{f}\xi) \in \mathbb{G}_f\}$. An equivalence of the two definitions is easily verified.

It is also easy to verify the following criterion.

Lemma 2.19. *Any set $\mathbb{G} \subset \mathbb{H}$ determines a linear operator $\hat{f}$ in $\mathfrak{H}$, i.e., $\mathbb{G} = \mathbb{G}_f$ iff $\mathbb{G}$ is a subspace with the property*

$$(0 \diagup \eta) \in \mathbb{G} \Longrightarrow \eta = 0 \tag{2.11}$$

ensuring that $\mathbb{G}$ be a graph ($\mathbb{G}_f$ is a "hyperplane" passing through the origin in $\mathfrak{H}$).

We call this criterion the *graph criterion* for a linear operator.

In the *language of graphs*, it is particularly evident that the definition of a linear operator $\hat{f}$ includes both the "rule of acting" and the domain of definition.

Many notions and theorems in the theory of linear operators are easily formulated and proved in terms of graphs; because we deal only with linear operators, we often omit the term "linear" in what follows.

The first example is the notion of equal operators: two operators $\hat{f}_1$ and $\hat{f}_2$ are equal, or coincide, written $\hat{f}_1 = \hat{f}_2$, if their graphs coincide, $\mathbb{G}_{f_1} = \mathbb{G}_{f_2}$. In the language of maps, this means that $D_{f_1} = D_{f_2}$ and $\hat{f}_1\xi = \hat{f}_2\xi$, $\forall\xi \in D_{f_1} = D_{f_2}$.

Another example is given by the important notions of extension and restriction of an operator. An operator $\hat{f}_2$ is called an *extension of an operator* $\hat{f}_1$, while $\hat{f}_1$ is called a *restriction of an operator* $\hat{f}_2$, if $G_{f_1} \subset G_{f_2}$, which is naturally written $\hat{f}_1 \subset \hat{f}_2$. In the *language of maps*, this means that $D_{f_1} \subset D_{f_2}$ and $\hat{f}_2\xi = \hat{f}_1\xi$, $\forall\xi \in D_{f_1}$. We say that the operator f_1 is a restriction of the operator $\hat{f}_2$ to the subspace $D_{f_1} \subset D_{f_2}$, while the operator f_2 is an extension of the operator $\hat{f}_1$ to the subspace $D_{f_2} \supset D_{f_1}$. Any operator $\hat{f}$ allows restricting to any subspace $D_g \subset D_f$, which defines a restriction $\hat{g}$ of the operator $\hat{f}$.

In what follows, we use both languages.

2.3.3 *Examples of Operators*

Examples of operators include the identity or unity operator $\hat{I}$:

$$\hat{I} : \mathfrak{H} \longrightarrow \mathfrak{H}\,,\ \ \hat{I}\xi = \xi\,,\ \ \forall\xi \in \mathfrak{H}\,,\ \ D_I = \mathfrak{H}\,,\ \ R_I = \mathfrak{H}\,,\ \ \mathbb{G}_I = \{(\xi \diagup \xi)\} = \operatorname{diag}\mathbb{H}\,,$$

and the multiple of unity operator $z\hat{I}$, $z \in \mathbb{C}$, $z \neq 0$:

$$z\hat{I} : \mathfrak{H} \longrightarrow \mathfrak{H}\,,\ (z\hat{I})\xi = z\xi\,,\ \ \forall\xi \in \mathfrak{H}\,,\ \ D_{zI} = \mathfrak{H}\,,\ \ R_{zI} = \mathfrak{H}\,,\ \mathbb{G}_{zI} = \{(\xi \diagup z\xi)\}\,.$$

It is evident that the multiple of unity operator maps any subspace onto the same subspace, $(z\hat{I})D = D$. With $z = 0$, we obtain the zero operator $\hat{0}$: $\mathfrak{H} \longrightarrow \{0\}$. The multiple of unity operator with $|z| \neq 1$ changes the lengths of vectors.

The momentum operator for a particle moving on the real axis is the operator $\hat{p} = -i\hbar d_x$ in $L^2(\mathbb{R})$; its domain D_p is the space of absolutely continuous functions square-integrable on the whole axis together with their derivatives,[12] $D_p = \{\psi(x) : \psi \text{ are a.c.}, \psi, \psi' \in L^2(\mathbb{R})\}$. This operator is an extension of the operator $\hat{p}^{(0)} = -i\hbar d_x$ with the same rule of action, but defined on the space of smooth functions with compact support, $D_{p^{(0)}} = \mathcal{D}(\mathbb{R})$, $\hat{p}^{(0)} \subset \hat{p}$. Other examples of differential operators in Hilbert spaces $L^2(a, b)$ are considered in detail in Chaps. 4 and 6.

Analogues of rotation in finite-dimensional spaces are isometric and unitary operators.

An operator $\hat{U}$ is called isometric if it preserves the norm of vectors, $\|\hat{U}\xi\| = \|\xi\|$, $\forall \xi \in D_U$, or, which is the same, if it preserves the scalar product of vectors, $(\hat{U}\xi, \hat{U}\eta) = (\xi, \eta)$, $\forall \xi, \eta \in D_U$. The equivalence of the two conditions follows from the chain of equalities

$$\begin{aligned}\left(\hat{U}(\xi + z\eta), \hat{U}(\xi + z\eta)\right) &= \left(\hat{U}\xi, \hat{U}\xi\right) + z\left(\hat{U}\xi, \hat{U}\eta\right) + \bar{z}\left(\hat{U}\eta, \hat{U}\xi\right) \\ &\quad + |z|^2\left(\hat{U}\eta, \hat{U}\eta\right) = (\xi + z\eta, \xi + z\eta) \\ &= (\xi, \xi) + z(\xi, \eta) + \bar{z}(\eta, \xi) + |z|^2(\eta, \eta).\end{aligned}$$

We say that the range and the domain of an isometric operator are related by an isometry relation, or simply by isometry; therefore, an isometric operator is also called an isometry. For completeness, we say in advance that an isometric operator is bounded and its norm is equal to unity, the corresponding notions are introduced in Sect. 2.3.4. It is evident that the domain and the range of an isometric operator $\hat{U}$ are of the same dimension, $\dim D_U = \dim R_U$. In contrast to the finite-dimensional case, this does not mean that if an isometric operator is defined everywhere, then its range must be all of $\mathfrak{H}$. A counterexample is the operator $\hat{U}$ first defined on an orthonormal basis $\{e_n\}_1^\infty$ by $\hat{U}e_n = e_{n+1}$ and then extended to any vector $\xi = \sum_1^\infty a_n e_n$ by linearity: $\hat{U}\xi = \sum_1^\infty a_n e_{n+1}$; it is evident that the operator is isometric, and $D_U = \mathfrak{H}$, while $R_U = \{ae_1, \forall a \in \mathbb{C}\}^\perp$, the orthogonal complement of the one-dimensional space spanned by the vector e_1.

An isometric operator $\hat{U}$ is called unitary if it is defined everywhere and maps $\mathfrak{H}$ onto the whole of $\mathfrak{H}$, $D_U = \mathfrak{H} = R_U$.

We cite some important properties of unitary operators that are used below and are easily verified.

Lemma 2.20. *(i) A unitary operator is bounded, and its norm is equal to unity.*

(ii) A unitary operator maps a closed set onto a closed set and commutes with the closure operation $^{-}$*:*

$$\hat{U}\overline{M} = \overline{\hat{U}\overline{M}} = \overline{\hat{U}M} \tag{2.12}$$

for any set $M \subseteq \mathfrak{H}$. In particular, a unitary operator maps a closed subspace onto a closed subspace, $\hat{U}\overline{D} = \overline{\hat{U}\overline{D}} = \overline{\hat{U}D}$.

[12] In what follows, we often omit the symbol for the argument of a function if it is clear from context.

(iii) *A unitary operator transforms an orthonormal basis* $\{e_i\}_1^\infty$ *to an orthonormal basis* $\{e_i'\}_1^\infty$ *and is completely determined by its action on an orthonormal basis,* $\hat{U}e_i = e_i'$, $i \in \mathbb{N}$.

(iv) *For any subspace* $D \subset \mathfrak{H}$*, a unitary operator transforms its orthogonal complement to the orthogonal complement of the image* $\hat{U}D$*, i.e., it commutes with the orthogonal complement operation* $^\perp$,

$$\hat{U}D^\perp = \left(\hat{U}D\right)^\perp . \tag{2.13}$$

(v) *A unitary operator commutes with the orthogonal direct sum operation* $\oplus$,

$$\mathfrak{H} = \hat{U}\mathfrak{H} = \hat{U}\left(\overline{D} \oplus D^\perp\right) = \hat{U}\overline{D} \oplus \hat{U}D^\perp = \overline{\hat{U}D} \oplus \left(\hat{U}D\right)^\perp .$$

A trivial example of a unitary operator is the unity operator $\hat{I}$. The simplest nontrivial example is the multiple of unity operator $\hat{U} = z\hat{I}$ with $z = \mathrm{e}^{\mathrm{i}\varphi}$, $0 \leq \varphi \leq 2\pi$.

We also introduce some simple "matrix" unitary operators Σ_1 and $\mathcal{E}$ in the composite Hilbert space $\mathbb{H}$ that are well known to physicists as the spin operators:

$$\Sigma_1 = \begin{pmatrix} 0 & \hat{I} \\ \hat{I} & 0 \end{pmatrix}, \; \Sigma_1(\xi/\eta) = (\eta/\xi)\,;$$

$$\mathcal{E} = i\Sigma_2 = \begin{pmatrix} 0 & \hat{I} \\ -\hat{I} & 0 \end{pmatrix}, \; \mathcal{E}(\xi/\eta) = (\eta/-\xi)\,. \tag{2.14}$$

The operators Σ_1 and $\mathcal{E}$ are evidently unitary and therefore commute with the closure operation and the orthogonal complement operation. These operators are extensively used below in defining the inverse and adjoint operators in terms of graphs.

2.3.4 Properties of Linear Operators

We now touch upon some general properties of operators. In general, an operator $\hat{f}$ rotates and stretches the vectors belonging to D_f. The measure of stretching is its norm $\|\hat{f}\|$ defined by

$$\left\|\hat{f}\right\| = \sup_{\xi \in D_f,\, \xi \neq 0} \left\|\hat{f}\xi\right\| \|\xi\|^{-1} = \sup_{\xi \in D_f,\, \|\xi\|=1} \left\|\hat{f}\xi\right\| . \tag{2.15}$$

It is evident that $\|\hat{f}\xi\| \leq \|\hat{f}\|\,\|\xi\|$, $\forall \xi \in D_f$, and

$$\left|(\eta, \hat{f}\xi)\right| \leq \left\|\hat{f}\right\| \|\xi\| \, \|\eta\| \,, \; \forall \xi \in D_f \,, \; \forall \eta \in \mathfrak{H} \,.$$

An operator $\hat{f}$ is called a *bounded operator* if its norm is finite, $\|\hat{f}\| < \infty$; otherwise, it is called an *unbounded operator*.

An operator $\hat{f}$ is called a *continuous operator* if

$$\xi \longrightarrow \xi_0, \; \xi, \xi_0 \in D_f \Longrightarrow \hat{f}\xi \longrightarrow \hat{f}\xi_0 \,.$$

The continuity of any operator is obviously equivalent to its continuity at the origin: $\xi \longrightarrow 0 \Longrightarrow \hat{f}\xi \longrightarrow 0$.

Some of the trivial examples of bounded and continuous operators are the multiple of unity operator $\hat{f} = z\hat{I}$, $\|\hat{f}\| = |z|$, and the unitary operator, $\hat{f} = \hat{U}$, $\|\hat{U}\| = 1$.

We list some well-known properties of bounded operators (see, for example, [9]).

Lemma 2.21. *(i) An operator $\hat{f}$ is continuous iff it is bounded.*

(ii) A continuous operator $\hat{f}$ can be extended by continuity to the closure $\overline{D_f}$ of the initial domain D_f with the same norm. If $\overline{D_f} \neq \mathfrak{H}$, an operator $\hat{f}$ can be extended to the whole of $\mathfrak{H}$ with the same norm[13] *(for example, by setting $\hat{f}D^{\perp} = \{0\}$).*

Bounded operators defined everywhere form an associative algebra with the natural operations of addition and multiplication respectively defined by

$$(a\hat{f} + b\hat{g})\xi = a\hat{f}\xi + b\hat{g}\xi \,, \; \forall \xi \in \mathfrak{H} \,, \; \forall a, b \in \mathbb{C} \,, \; (\hat{f}\hat{g})\xi = \hat{f}(\hat{g}\xi),$$

and obeying the distributive law:

$$(\hat{f} + \hat{g})\hat{h} = \hat{f}\hat{h} + \hat{g}\hat{h}, \;\; \hat{h}(\hat{f} + \hat{g}) = \hat{h}\hat{f} + \hat{h}\hat{g}.$$

In particular, the commutator of two bounded operators is well defined.

This algebra is normed with the previously defined norm $\|\hat{f}\|$, which fulfills the standard requirements for a norm and also has the property $\|\hat{f}\hat{g}\| \leq \|\hat{f}\|\|\hat{g}\|$. The distance between two operators $\hat{f}$ and $\hat{g}$ is defined as $\|\hat{f} - \hat{g}\|$; it determines the so-called uniform operator topology, similar to the strong topology in $\mathfrak{H}$. A sequence $\{\hat{f}_n\}_1^{\infty}$ of operators is called uniformly convergent to an operator $\hat{f}$, written $\hat{f}_n \overset{n\to\infty}{\Longrightarrow} \hat{f}$, if $\|\hat{f}_n - \hat{f}\| \overset{n\to\infty}{\longrightarrow} 0$. As a linear space the algebra is complete with respect to the uniform operator topology.

Along with uniform convergence, two other kinds of convergence, namely, *strong operator convergence* and *weak operator convergence*, are introduced for bounded operators defined everywhere. A sequence $\{\hat{f}_n\}_1^{\infty}$ of operators is called strongly

[13] An unbounded operator cannot in general be defined in all of $\mathfrak{H}$.

convergent to an operator $\hat{f}$, written $\hat{f}_n \overset{n\to\infty}{\longrightarrow} \hat{f}$, if $\hat{f}_n\xi \overset{n\to\infty}{\longrightarrow} \hat{f}\xi$, $\forall\xi \in \mathfrak{H}$, and weakly convergent to an operator $\hat{f}$, written $\hat{f}_n \overset{w}{\to} \hat{f}$, if $\mathrm{wlim}_{n\to\infty}\hat{f}_n\xi = \hat{f}\xi$, $\forall\xi \in \mathfrak{H}$. Strong convergence follows from uniform convergence, and weak convergence follows from strong convergence and a fortiori from uniform convergence.

A bounded operator $\hat{f}$ generates a bounded sesquilinear form w_f defined by

$$w_f(\eta,\xi) = \left(\eta, \hat{f}\xi\right), \ \left|w_f(\eta,\xi)\right| \le \left\|\hat{f}\right\| \|\eta\| \|\xi\|,$$

and $\hat{f}$ is completely determined by w_f. Moreover, $\hat{f}$ is completely determined by its matrix elements $f_{mn} = (e_m, \hat{f}e_n)$ with respect to any orthonormal basis $\{e_n\}_1^\infty$. In this sense, bounded operators are similar to finite-dimensional operators.

The algebraic situation with unbounded operators is more involved because of generally different domains and ranges for different operators.

The multiplication of an unbounded operator $\hat{f}$ by a complex number $z \in \mathbb{C}$ is naturally defined by $(z\hat{f})\xi = z\hat{f}\xi$, $\xi \in D_{zf} = D_f$. But the sum and product of two unbounded operators $\hat{f}$ and $\hat{g}$ with the respective domains D_f and D_g are more involved. They are respectively defined by

$$\left(\hat{f} + \hat{g}\right)\xi = \hat{f}\xi + \hat{g}\xi, \ \xi \in D_{f+g} = D_f \cap D_g,$$

and

$$\left(\hat{f}\hat{g}\right)\xi = \hat{f}(\hat{g}\xi), \ \xi \in D_{fg} = \left\{\xi : \xi \in D_g, \ \hat{g}\xi \in D_f\right\}.$$

If $\hat{f}$ or $\hat{g}$ is defined everywhere, $D_f = \mathfrak{H}$ or $D_g = \mathfrak{H}$, then we respectively have $D_{f+g} = D_g$ or $D_{f+g} = D_f$. In particular, the domain of the operator $\hat{f} - z\hat{I}$ is $D_{f-zI} = D_f$, so that $\hat{f} - z\hat{I} = \hat{f} - z\hat{I}_{D_f}$, where $\hat{I}_{D_f}$ is the restriction of the identity operator $\hat{I}$ to D_f.

It may be that $D_f \cap R_g = \{0\}$, in which case the product $\hat{f}\hat{g}$ is defined on only the zero subspace, but if $D_f = \mathfrak{H}$, then $D_{fg} = D_g$.

As to the distributive law, we have the equality

$$(\hat{f} + \hat{g})\hat{h} = \hat{f}\hat{h} + \hat{g}\hat{h} \tag{2.16}$$

and in general, the inclusion $\hat{h}(\hat{f} + \hat{g}) \supseteq \hat{h}\hat{f} + \hat{h}\hat{g}$, but if $\hat{h}$ is defined everywhere, the inclusion becomes an equality:

$$\hat{h}(\hat{f} + \hat{g}) = \hat{h}\hat{f} + \hat{h}\hat{g}, \text{ if } D_h = \mathfrak{H}. \tag{2.17}$$

We see that there is no natural associative algebra for arbitrary operators, notably unbounded ones. In particular, a notion of commutativity cannot be naturally defined for two arbitrary operators. But if at least one of two operators $\hat{f}$ and $\hat{g}$ is defined everywhere, let it be $\hat{f}$, $D_f = \mathfrak{H}$, then we say that these operators commute if $\hat{f}\hat{g} \subseteq \hat{g}\hat{f}$, i.e., the product $\hat{g}\hat{f}$ is an extension of the product $\hat{f}\hat{g}$, which means that

$\hat{f}\xi \in D_g$, $\forall\xi \in D_g$ and $\hat{f}\hat{g}\xi = \hat{g}\hat{f}\xi$. We note that this notion of commutativity is extensively used in QM in defining the symmetry of unbounded observables $\hat{g}$ under unitarily implemented group transformations $\hat{f} = \hat{U}$. In QM, a commutativity of observables is also extensively used; we say in advance that for s.a. operators, commutativity can be defined by reducing to the case of bounded operators.

Remark 2.22. An unbounded operator is not generally determined by its matrix $\{f_{mn}\}$ with respect to an orthonormal basis $\{e_n\}_1^\infty$ even if $e_n \in D_f$, $\forall n$, and the matrix does exist (an example is given below). Therefore, any operations with unbounded operators, in particular definitions of the adjoint operator, and consequently of self-adjointness, in terms of the corresponding matrices are generally improper. In relativistic quantum field theory, a situation with observables and with a proper formulation of the theory itself is more involved and even dramatic. For example, in the relativistic local $\lambda\varphi^4$-theory of a scalar field φ in $3+1$ dimensions, the Hamiltonian $\hat{H}$ in the Fock space is formally given by

$$\begin{aligned}\hat{H} &=: \int d\mathbf{x} \left\{ \frac{1}{2}\hat{\pi}^2(\mathbf{x}) + (\nabla\hat{\varphi})^2(\mathbf{x}) + m^2\hat{\varphi}^2(\mathbf{x}) + \frac{\lambda}{4!}\hat{\varphi}^4(\mathbf{x}) \right\}: \\ &= \int d\mathbf{k}\omega(\mathbf{k})\hat{a}^+(\mathbf{k})\hat{a}(\mathbf{k}) + \frac{\lambda}{4!(2\pi)^3}\int \frac{d\mathbf{k}_1\cdots d\mathbf{k}_4}{\sqrt{2\omega(\mathbf{k}_1)\cdots 2\omega(\mathbf{k}_4)}} \\ &\quad \times [\hat{a}^+(\mathbf{k}_1)\cdots\hat{a}^+(\mathbf{k}_4)\delta^3(\mathbf{k}_1+\cdots+\mathbf{k}_4)+\cdots],\ \omega(\mathbf{k}) = \sqrt{\mathbf{k}^2+m^2},\end{aligned}$$

where $\hat{\pi}$ is the canonical momentum operator, and $\hat{a}^+, \hat{a}$ are the conventional creation and annihilation operators. But this $\hat{H}$ actually defines only a sesquilinear form $(\psi, \hat{H}\phi)$ on the linear envelope of terminating Fock vectors, or a matrix in the (generalized) orthonormal basis $\frac{1}{n!}\hat{a}^+(\mathbf{k}_1)\cdots\hat{a}^+(\mathbf{k}_n)\hat{\phi}_0$, where $\hat{\phi}_0$ is the Fock vacuum, and not an operator: $\hat{H}$ has no nontrivial domain of definition because of the volume and ultraviolet divergences. To be defined, $\hat{H}$ requires some volume and ultraviolet cutoffs; this is the subject matter of constructive field theory.

After this remark, we turn to properties of unbounded operators. An analogue of continuity for unbounded operators that is sufficient in many cases is *closedness*.

An operator $\hat{f}$ is called a *closed operator*, written $\hat{f} = \overline{\hat{f}}$ (the notation becomes clear below), if its graph is closed (as a subspace in $\mathbb{H}$), $\mathbb{G}_f = \overline{\mathbb{G}_f}$.

A weakened version of closedness is *closability*. An operator $\hat{f}$ is called a *closable operator* if the closure $\overline{\mathbb{G}_f}$ of its graph $\mathbb{G}_f$ in $\mathbb{H}$ is also a graph, and therefore determines the operator $\overline{\hat{f}}$, which is called the *closure* of $\hat{f}$.

For a closable operator $\hat{f}$, we have $\hat{f} \subseteq \overline{\hat{f}}$; a closed operator is a trivial particular case of a closable operator that coincides with its closure, $\hat{f} = \overline{\hat{f}}$. Therefore, when we use the term "closable operator" in what follows, we as a rule actually mean a "closable, in particular closed, operator," which is explicitly represented in formulas by the symbol $\subseteq$.

It is easy to see that an operator $\hat{f}$ is closable if it has a closed extension $\hat{g} = \overline{\hat{g}}$: $\mathbb{G}_f \subset \mathbb{G}_g = \overline{\mathbb{G}_g}$ implies that $\overline{\mathbb{G}_f} \subseteq \mathbb{G}_g$, whence it follows that $\overline{\mathbb{G}_f}$ is a graph, the graph of the closure $\overline{\hat{f}}$, which is evidently the minimum closed extension of a closable $\hat{f}$.

In the language of maps, definitions of these notions are more lengthier. An operator $\hat{f}$ is called closed if the simultaneous realization of the two relations

$$\lim_{n\to\infty} \xi_n = \xi, \ \lim_{n\to\infty} \hat{f}\xi_n = \eta, \ \forall \xi_n \in D_f,$$

implies that $\xi \in D_f$ and $\hat{f}\xi = \eta$.

An operator is called closable, or has a closure, if the simultaneous realization of the relations

$$\lim_{n\to\infty} \xi_n = \lim_{n\to\infty} \xi_n' = \xi, \ \lim_{n\to\infty} \hat{f}\xi_n = \eta, \ \lim_{n\to\infty} \hat{f}\xi_n' = \eta', \quad \forall \xi_n, \xi_n' \in D_f,$$

implies that $\eta = \eta'$.

The difference between continuous and closed operators is that if $\hat{f}$ is continuous (bounded) then $\xi_n \longrightarrow \xi$ implies that[14] $\hat{f}\xi_n \longrightarrow \eta$, while if $\hat{f}$ is only closed, the sequence $\{\hat{f}\xi_n\}_1^\infty$ can diverge (for an unbounded $\hat{f}$). But in both cases, a situation in which $\xi_n^{(1)} \longrightarrow \xi, \ \xi_n^{(2)} \longrightarrow \xi$ and simultaneously $\hat{f}\xi_n^{(1)} \longrightarrow \eta^{(1)}, \ \hat{f}\xi_n^{(2)} \longrightarrow \eta^{(2)}$ with $\eta^{(1)} \neq \eta^{(2)}$ is forbidden.

The latter is a necessary and sufficient condition for closability. An equivalent criterion for closability directly follows from the graph criterion (2.11), Lemma 2.19: an operator $\hat{f}$ is closable iff the simultaneous realization of the relations $\xi_n \longrightarrow 0$, $\xi_n \in D_f$, and $\hat{f}\xi_n \longrightarrow \eta$ implies that $\eta = 0$. The closure $\overline{\hat{f}}$ of a closable operator $\hat{f}$ now can be described in terms of sequences as follows: a vector ξ belongs to the domain $D_{\overline{f}}$ of $\overline{\hat{f}}$ iff there exists a sequence of vectors $\{\xi_n\}_1^\infty$, $\xi_n \in D_f$, so that if $\xi_n \longrightarrow \xi$ and $\hat{f}\xi_n \longrightarrow \eta$, then $\overline{\hat{f}}\xi = \eta$.

For a continuous operator, the relation $\xi_n \longrightarrow 0$ implies that $\hat{f}\xi_n \longrightarrow 0$, and therefore, any continuous operator $\hat{f}$ is closable, its closure $\overline{\hat{f}}$ is also continuous, and $\|\hat{f}\| = \|\overline{\hat{f}}\|$. For future reference, the following assertion is formulated as a lemma.

Lemma 2.23. *The domain of a closed continuous (bounded) operator $\hat{f}$, $\hat{f} = \overline{\hat{f}}$, is closed, $D_f = \overline{D_f}$, i.e., D_f is either a closed subspace in $\mathfrak{H}$ or the whole of $\mathfrak{H}$, and conversely, if $D_f = \overline{D_f}$, a continuous operator $\hat{f}$ is closed, $\hat{f} = \overline{\hat{f}}$.*

[14] It may be that $\xi \notin D_f$ if $\hat{f}$ is not closed; a continuous $\hat{f}$ can be nonclosed, but is always closable (see below).

In part, this assertion is a paraphrase of the above-cited assertion that a continuous operator allows extending by continuity to the closure of its domain. We note that in general, the range of a continuous operator is not necessarily closed.

In contrast to continuous operators, not every unbounded operator has a closure. Of course, any graph $\mathbb{G}_f$ is closable, but the closure $\overline{\mathbb{G}_f}$ may be not a graph.

A counterexample is the operator $\hat{f}$ in $L^2(0,\pi)$ defined on the subspace of all continuous functions and given by

$$\hat{f}\psi(x) = \psi(0)\sin x. \tag{2.18}$$

This operator is evidently densely defined and unbounded. For the sequence $\{\psi_n(x) = \mathrm{e}^{-nx}\}_1^\infty$ of continuous functions, we have $\psi_n \longrightarrow 0$, but $\hat{f}\psi_n(x) = \sin x \neq 0$. It follows that this operator is nonclosable, and a fortiori nonclosed.

The characteristic property of a nonclosable operator is that its matrix $\{f_{mn}\}$ with respect to an orthonormal basis $\{e_n\}_1^\infty$ does not determine the operator. Taking the orthonormal basis $\left\{e_n = \sqrt{2/\pi}\sin nx\right\}_1^\infty$ in the above example, we have $f_{mn} \equiv 0$, whereas $\hat{f} \neq 0$.

For a closed unbounded operator $\hat{f}$, neither its domain D_f nor, in general, its range R_f is a closed subspace.

Remark 2.24. QM observables must be closed operators. This is clear from the physical considerations related to the inaccuracy of measurement: the inaccuracy in determining a state must have no strong effect on measurable observables. On the other hand, QM observables must be densely defined.

There is no strong relation between the closure operation and algebra of unbounded operators. It is evident that if an operator $\hat{f}$ is closable, then the operator $a\hat{f}$, $\forall a \in \mathbb{C}$, is also closable, and $\overline{a\hat{f}} = a\overline{\hat{f}}$. As to the closability and closure of the sum and product of closable operators, we cannot say something definite in the general case. For example, the sum of two closed operators may be nonclosed, and the same holds for their product. But if one of the two closable operators $\hat{f}$ and $\hat{g}$ is bounded and defined everywhere, and is therefore closed, let it be $\hat{g}$, $\hat{g} = \overline{\hat{g}}$, then their sum is closable, and the closure of the sum is the sum of the corresponding closures, $\overline{\hat{f} + \hat{g}} = \overline{\hat{f}} + \hat{g}$. In particular, if an operator $\hat{f}$ is closable, then the operator $\hat{f} - z\hat{I}$ is also closable, and

$$\overline{\hat{f} - z\hat{I}} = \overline{\hat{f}} - z\hat{I}, \quad \forall z \in \mathbb{C}. \tag{2.19}$$

Under the same conditions, the product $\hat{f}\hat{g}$ is closable, and $\hat{f}\hat{g} \subseteq \overline{\hat{f}\hat{g}} = \overline{\hat{f}}\hat{g}$. A condition on $\hat{f}$ under which the product $\hat{f}\hat{g}$ is closable is given below.

2.3.4.1 Examples of Unbounded Operators

As an example, we consider the differentiation operator $\hat{d}_x$ in the Hilbert space $L^2(a,b)$,

$$\hat{d}_x : \begin{cases} D_d = \{\psi(x) :\ \psi \text{ a.c. in } (a,b),\ \psi, \psi' \in L^2(a,b)\}, \\ \hat{d}_x \psi(x) = \psi'(x). \end{cases}$$

We show that the operator $\hat{d}_x$ is unbounded for any interval $(a,b) \subseteq \mathbb{R}$.

Let $(a,b) = [0,1]$. We consider the sequence $\{\psi_n\}_1^\infty$ of functions of unit norm,

$$\psi_n(x) = [2(1+1/n)]^{1/2} x^{1/2+1/n},\ \ \|\psi_n\|^2 = 2(1+1/n)\int_0^1 x^{2(1/2+1/n)} \mathrm{d}x = 1.$$

It is easy to see that

$$\hat{d}_x \psi_n(x) = \psi_n'(x) = (1/2+1/n)[2(1+1/n)]^{1/2} x^{-1/2+1/n},$$
$$\|\psi_n'\|^2 = (1/2+1/n)^2(1+1/n)n = n/4 + O(1),$$

whence it follows that the functions ψ_n with any n belong to the domain D_d of the operator $\hat{d}_x$ and its norm is estimated from below by $\|\hat{d}_x\| > n/4$, where n is arbitrarily large, which means that $\hat{d}_x$ is an unbounded operator. The operator $\hat{d}_x$ cannot be defined on the whole of $L^2(0,1)$; for example, it is not defined on functions $\psi_\alpha = x^\alpha$, $-1/2 < \alpha \le 1/2$: although $\psi_\alpha \in L^2(0,1)$, we have $\psi_\alpha' \notin L^2(0,1)$ because $\|\psi_\alpha'\|^2 = \infty$.

The same conclusions hold for the operators $\hat{d}_x$ in $L^2(\mathbb{R}_+)$ and $L^2(\mathbb{R})$ due to similar arguments.

By similar arguments, similar conclusions hold for the double differentiation operator with the rule of action d_x^2.

It can be shown that the operator of multiplication by the independent variable x in $L^2(\mathbb{R}_+)$ and $L^2(\mathbb{R})$ is unbounded, whereas in $L^2(a,b)$, $|a|, |b| < \infty$, it is bounded, see Sect. 4.3.3.

We now turn to the notions and properties of inverse and adjoint operators, which are of great importance in what follows.[15] These notions are most easily defined and described in the language of graphs via the above-introduced unitary transformations Σ_1 and $\mathcal{E}$ (2.14) in $\mathbb{H}$.

[15] In particular, criteria for closability and methods for constructing the closure are formulated in terms of them.

2.4 Inverse Operator

As a preliminary step, we need the important notion of the kernel of an operator. By definition, the *kernel of an operator* $\hat{f}$ (or null space),[16] denoted by $\ker \hat{f}$, is the eigenspace of $\hat{f}$ corresponding to the zero eigenvalue: $\ker \hat{f} = \{\xi : \xi \in D_f, \hat{f}\xi = 0\}$. For a closed $\hat{f}$, its kernel is a closed subspace: $\hat{f} = \overline{\hat{f}} \Longrightarrow \ker \hat{f} = \overline{\ker \hat{f}}$.

It is evident that the eigenspace of an operator $\hat{f}$ corresponding to the eigenvalue λ can be defined as $\ker(\hat{f} - \lambda\hat{I})$; λ is an eigenvalue of $\hat{f}$ iff $\ker(\hat{f} - \lambda\hat{I}) \neq \{0\}$.

2.4.1 Definition and Properties

We now consider the action of the unitary operator Σ_1 in $\mathbb{H} = \mathfrak{H} \oplus \mathfrak{H}$ on the graph $\mathbb{G}_f = \{(\xi/\eta = \hat{f}\xi)\} \subset \mathbb{H}$ of an operator $\hat{f}$. The natural question arises whether the subspace $\Sigma_1\mathbb{G}_f = \{(\eta = \hat{f}\xi/\xi)\} \subset \mathbb{H}$ (with transposed abscissas and ordinates) is a graph in itself and therefore determines some operator.

Definition 2.25. An operator $\hat{f}$ is called invertible if the subspace $\Sigma_1\mathbb{G}_f \subset \mathbb{H}$ is a graph. If so, this graph determines the operator called the inverse operator, or simply the inverse, of $\hat{f}$, which is denoted by $\hat{f}^{-1}$, such that $\xi = \hat{f}^{-1}\eta$,

$$\mathbb{G}_{f^{-1}} = \Sigma_1\mathbb{G}_f = \left\{\left(\eta/\xi = \hat{f}^{-1}\eta\right)\right\}.$$

A criterion for invertibility follows from the graph criterion (2.11), Lemma 2.19: an operator $\hat{f}$ is invertible and the inverse operator $\hat{f}^{-1}$ exists iff $\eta = \hat{f}\xi = 0 \Longrightarrow \xi = 0$, or $\hat{f}$ has the zero kernel, $\ker \hat{f} = \{0\}$. An evident generalization of this assertion is that an operator $\hat{f} - z\hat{I}$, $z \in \mathbb{C}$, is invertible and its inverse $(\hat{f} - z\hat{I})^{-1}$ exists iff $\ker(\hat{f} - z\hat{I}) = 0$, or z is not an eigenvalue of $\hat{f}$. Conversely, if λ is an eigenvalue of $\hat{f}$, then the operator $(\hat{f} - \lambda\hat{I})^{-1}$ does not exist, and vice versa.

In the language of maps, if $\ker \hat{f} = \{0\}$, then there is a one-to-one correspondence between any $\xi \in D_f$ and $\eta = \hat{f}\xi \in R_f$, and the operator $\hat{f}$ has the inverse operator $\hat{f}^{-1}$ that maps $\eta = \hat{f}\xi$ to ξ, $\xi = \hat{f}^{-1}\eta$. We call the operation $^{-1}$ that assigns the inverse operator $\hat{f}^{-1}$ to every invertible operator $\hat{f}$, $\hat{f} \xrightarrow{-1} \hat{f}^{-1}$, the inversion operation.

The invertibility of an operator $\hat{f}$ implies that the equation $\hat{f}\xi = \eta$, $\xi \in D_f$, $\eta \in R_f$ is resolvable uniquely: $\xi = \hat{f}^{-1}\eta$.

We cite the properties of an inverse operator, which are easily verified.

[16] The latter term is used to avoid confusion with the kernel of an integral operator.

Lemma 2.26. *For any invertible operator $\hat{f}$, the following relations hold:*

(i) $\hat{f}^{-1}$ *is invertible, i.e.,* $\ker \hat{f}^{-1} = \{0\}$, *and* $\left(\hat{f}^{-1}\right)^{-1} = \hat{f}$ *(because* $\Sigma_1^2 = \widehat{\mathbb{I}}$, *the identity operator in* $\mathbb{H}$*).*

(ii) $\hat{f}^{-1}\hat{f} = \hat{I}_{D_f}, \hat{f}\hat{f}^{-1} = \hat{I}_{R_f}$, *where* $\hat{I}_{D_f}$ *and* $\hat{I}_{R_f}$ *are the restrictions of the identity operator* $\hat{I}$ *to the respective subspaces* D_f *and* R_f.

(iii) $D_{f^{-1}} = R_f, \quad R_{f^{-1}} = D_f$.

(iv) $\left\|\hat{f}\right\| \left\|\hat{f}^{-1}\right\| \geq 1\,.$

As an example, an isometric (unitary) operator $\hat{U}$ is invertible and $\hat{U}^{-1}$ is also isometric (unitary).

The following are the connections between the notion of invertibility and the previously defined notions of boundedness, extension, closability, and algebra.

2.4.2 Invertibility and Boundedness

Lemma 2.27. *If* $\|\hat{f}\,\xi\| \geq c\|\xi\|,\ c > 0$, *then* $\hat{f}$ *is invertible and* $\hat{f}^{-1}$ *is bounded:* $\|\hat{f}^{-1}\| \leq c^{-1}$. *The converse also holds.*

Proof. The inequality $\|\hat{f}\xi\| \geq c\|\xi\|$, $c > 0$, evidently implies that $\ker \hat{f} = \{0\}$ and therefore $\hat{f}$ is invertible. The equality $\eta = \hat{f}\hat{f}^{-1}\eta$, $\forall \eta \in D_{f^{-1}}$, then implies $\|\eta\| = \|\hat{f}\hat{f}^{-1}\eta\| \geq c\|\hat{f}^{-1}\eta\|$. It follows that

$$\left\|\hat{f}^{-1}\eta\right\| \|\eta\|^{-1} \leq c^{-1},\ \forall \eta \in D_{f^{-1}},\ \eta \neq 0,$$

which means that $\|\hat{f}^{-1}\| \leq c^{-1}$. The converse is proved similarly using the equality $\xi = \hat{f}^{-1}\hat{f}\xi\,,\ \forall \xi \in D_f\,.$ □

2.4.3 Invertibility, Extension, and Closability

It is evident, especially in the language of graphs, that if an operator $\hat{f}$ allows an invertible extension, $\hat{f} \subset \hat{g}$, $\ker \hat{g} = \{0\}$, then $\hat{f}$ is also invertible and $\hat{f}^{-1}$ allows an invertible extension $\hat{f}^{-1} \subset \hat{g}^{-1}$.

For a closable operator, the relation between its inverse and the inverse of its closure is more specific.

Lemma 2.28. *Let an invertible operator be closable,* $\hat{f} \subseteq \overline{\hat{f}}$, *and let its inverse* $\hat{f}^{-1}$ *also be closable,* $\hat{f}^{-1} \subseteq \overline{\hat{f}^{-1}}$. *Then its closure* $\overline{\hat{f}}$ *is invertible, and* $\left(\overline{\hat{f}}\right)^{-1} = \overline{\hat{f}^{-1}}$. *Conversely, let* $\hat{f}$ *be a closable operator, and let its closure* $\overline{\hat{f}}$ *be invertible. Then* $\hat{f}$ *is invertible, its inverse* $\hat{f}^{-1}$ *is closable, and* $\overline{\hat{f}^{-1}} = \left(\overline{\hat{f}}\right)^{-1}$.

Proof. The lemma can be formulated as follows: for a closable operator $\hat{f}$, the equality $\left(\overline{\hat{f}}\right)^{-1} = \overline{\hat{f}^{-1}}$ holds if one of its sides, left-hand side or right-hand side, has a sense, i.e., the closure operation $^{-}$ and the inversion operation $^{-1}$ commute. This is a direct consequence of the commutativity of the closure operation and the unitary transformation Σ_1, which yields the following chain of equalities:

$$\mathbb{G}_{(\overline{f})^{-1}} = \Sigma_1 \mathbb{G}_{\overline{f}} = \Sigma_1 \overline{\mathbb{G}_f} = \overline{\Sigma_1 \mathbb{G}_f} = \overline{\mathbb{G}_{f^{-1}}} = \mathbb{G}_{\overline{f^{-1}}}.$$

The direct and converse assertions of the first part of the lemma are proved by respectively reading these equalities from left to right and from right to left. □

It may be that $\hat{f}$ is invertible, but its closure $\overline{\hat{f}}$ is not. For example, let $\{e_n\}_1^\infty$ be an orthonormal basis in $\mathfrak{H}$, and let η be a unit vector of the form

$$\eta = \sum_1^\infty a_n e_n, \ \forall a_n \neq 0, \ \|\eta\|^2 = \sum_1^\infty |a_n|^2 = 1.$$

The operator $\hat{f}$ densely defined on $D_f = L(\{e_n\}_1^\infty)$ and given by $\hat{f}\xi = \xi - (\eta, \xi)\eta$ is bounded:

$$\|\hat{f}\xi\|^2 = \|\xi\|^2 - |(\eta, \xi)|^2 \Longrightarrow \|\hat{f}\| = 1,$$

and therefore is closable, but is not closed, by Lemma 2.23, because D_f is not a closed subspace. It is easy to see that $\ker \hat{f} = \{0\}$ because the equality $\xi - (\eta, \xi)\eta = 0$ is impossible for a nonzero $\xi \in D_f$, a finite linear combination of basis vectors, and therefore, the operator $\hat{f}$ is invertible. The closure $\overline{\hat{f}}$ of $\hat{f}$ is defined everywhere and is given by the same formula, while its kernel is the one-dimensional subspace $\{a\eta, \ \forall a \in \mathbb{C}\}$ spanned by the vector η. Because $\ker \overline{\hat{f}} \neq \{0\}$, the operator $\overline{\hat{f}}$ is not invertible.

Changing $\hat{f}$ to $\hat{f}^{-1}$ and $\hat{f}^{-1}$ to $\hat{f} = (\hat{f}^{-1})^{-1}$ in the second part of Lemma 2.28 provides a useful criterion for closability and a method for constructing the closure: Let an operator $\hat{f}$ be invertible, and let its inverse $\hat{f}^{-1}$ be bounded, $\|\hat{f}^{-1}\| < \infty$, and therefore closable. Then $\hat{f}$ is closable if the closure $\overline{\hat{f}^{-1}}$ of the inverse is invertible, and $\overline{\hat{f}} = \left(\overline{\hat{f}^{-1}}\right)^{-1}$.

Because operators $\hat{f}$ and $\hat{f} - z\hat{I}$, $z \in \mathbb{C}$, are closable or nonclosable simultaneously and $\overline{\hat{f} - z\hat{I}} = \overline{\hat{f}} - z\hat{I}$, see (2.19), these criteria and method can be used with the operator $\hat{f}$ replaced by the operator $\hat{f} - z\hat{I}$ for some z.

For future reference, we combine some parts of Lemmas 2.23 and 2.28 into a separate lemma.

Lemma 2.29. *If an operator $\hat{f}$ is closed and invertible, then its inverse $\hat{f}^{-1}$ is also closed. If, in addition, the inverse $\hat{f}^{-1}$ is bounded, then the range R_f of the operator $\hat{f}$, which is the domain $D_{f^{-1}}$ of the inverse $\hat{f}^{-1}$, is closed; $R_f = D_{f^{-1}} = \overline{D_{f^{-1}}} = \overline{R_f}$, i.e., R_f is either a closed subspace in $\mathfrak{H}$ or the whole of $\mathfrak{H}$.*

The first assertion of the lemma is the second assertion of Lemma 2.28 related to a closed operator $\hat{f} = \overline{\hat{f}} : \hat{f}^{-1} = \overline{\hat{f}^{-1}}$. The second assertion is the first assertion of Lemma 2.23: $R_f = D_{f^{-1}}$ is a closed set as the domain of the closed bounded operator $\hat{f}^{-1}$.

2.4.4 Inversion Operation and Algebra

Lemma 2.30. *If an operator $\hat{f}$ is invertible and a number a is not equal to zero, $a \neq 0$, then the operator $a\hat{f}$ is also invertible and $(a\hat{f})^{-1} = a^{-1}\hat{f}^{-1}$. If operators $\hat{f}$ and $\hat{g}$ are invertible, then their product $\hat{f}\hat{g}$ is invertible, $(\hat{f}\hat{g})^{-1} = \hat{g}^{-1}\hat{f}^{-1}$, and*

$$D_{fg} = \hat{g}^{-1}\left(R_g \cap D_f\right), \; R_{fg} = \hat{f}\left(R_g \cap D_f\right).$$

We leave the proof to the reader.

We can also make a promised addition concerning the closability of the product of two operators. Let $\hat{g}$ be a closable operator, let $\hat{f}$ be an invertible operator, and let its inverse $\hat{f}^{-1}$ be a bounded operator defined everywhere and therefore closed, so that the operator $\hat{f} = (\hat{f}^{-1})^{-1}$ is also closed by Lemma 2.29. Then the product $\hat{f}\hat{g}$ is closable, and $\overline{\hat{f}\hat{g}} = \hat{f}\overline{\hat{g}}$. We leave the proof to the reader (it is based on the existence of the continuous inverse $\hat{f}^{-1}$).

As to the invertibility of the sum $\hat{f}+\hat{g}$ of two operators, we cannot say something definite in the general case (for example, let $\hat{g} = -\hat{f}$). A useful exception is given by the following lemma.

Lemma 2.31. *Let an operator $\hat{f}$ be bounded with $\|\hat{f}\| = c < 1$ and defined everywhere, $D_f = \mathfrak{H}$. Then the operator $\hat{I} - \hat{f}$ is invertible; the inverse $(\hat{I} - \hat{f})^{-1}$ is bounded, $\|(\hat{I} - \hat{f})^{-1}\| < (1-c)^{-1}$, and is also defined everywhere, $D_{(I-f)^{-1}} = R_{I-f} = \mathfrak{H}$; and it is given by $(\hat{I} - \hat{f})^{-1} = \sum_{k=0}^{\infty} \hat{f}^k$, where the series on the right-hand side is uniformly convergent (the operator analogue of the formula for the sum of a geometric progression).*

Proof. A proof of the first assertion of the lemma follows from the triangle inequality

$$\left\|(\hat{I} - \hat{f})\xi\right\| \geq \|\xi\| - \left\|\hat{f}\xi\right\| \geq (1-c)\,\|\xi\|\,, \;\forall \xi \in \mathfrak{H},$$

and then from Lemma 2.27. The proof of the second and third assertions is based on the evident equality

$$(\hat{I} - \hat{f}) \sum_{k=0}^{n} \hat{f}^k = \hat{I} - \hat{f}^{n+1}. \tag{2.20}$$

We first note that the operator sequence $\{\hat{f}^{n+1}\}_0^\infty$ uniformly converges to the zero operator: $\hat{f}^{n+1} \overset{n\to\infty}{\longrightarrow} \hat{0}$, because

$$\left\| \hat{f}^{n+1} \right\| \leq \left\| \hat{f} \right\|^{n+1} = c^{n+1} \overset{n\to\infty}{\longrightarrow} 0,$$

and a fortiori, it converges strongly: $\hat{f}^{n+1}\xi \overset{n\to\infty}{\longrightarrow} 0$, $\forall \xi \in \mathfrak{H}$. Second, the operator $\hat{f}$ is evidently closed, and therefore, the operator $\hat{I} - \hat{f}$ is also closed. Then by virtue of Lemma 2.29, its range R_{I-f} is a closed subspace, $R_{I-f} = \overline{R_{I-f}}$. Let a vector η belong to $(R_{I-f})^\perp$, the orthogonal complement of R_{I-f}, i.e., $(\eta, (\hat{I} - \hat{f})\xi) = 0$, $\forall \xi \in \mathfrak{H}$. Then (2.20) yields

$$(\eta, (\hat{I} - \hat{f}^{n+1})\xi) = (\eta, \xi) - (\eta, \hat{f}^{n+1}\xi) = 0, \quad \forall \xi \in \mathfrak{H}.$$

Passing to the limit $n \longrightarrow \infty$ in the last equality and using that $\hat{f}^{n+1}\xi \longrightarrow 0$ in this limit, we obtain $(\eta, \xi) = 0$, $\forall \xi \in \mathfrak{H}$, whence it follows that $\eta = 0$. This means that $(R_{I-f})^\perp = \{0\}$, and therefore, $R_{I-f} = \overline{R_{I-f}} = \mathfrak{H}$, which proves the second assertion. Multiplying (2.20) by $(\hat{I} - \hat{f})^{-1}$ from the left, we obtain

$$\left(\hat{I} - \hat{f}\right)^{-1} - \sum_{k=0}^{n} \hat{f}^k = \left(\hat{I} - \hat{f}\right)^{-1} \hat{f}^{n+1},$$

whence it follows that

$$\left\| \left(\hat{I} - \hat{f}\right)^{-1} - \sum_{k=0}^{n} \hat{f}^k \right\| = \left\| \left(\hat{I} - \hat{f}\right)^{-1} \hat{f}^{n+1} \right\| \leq c^{n+1} (1-c)^{-1} \overset{n\to\infty}{\longrightarrow} 0,$$

which proves the third assertion. □

2.5 Spectrum of an Operator

An important notion of the spectrum of an operator $\hat{f}$ is formulated in terms of the operator $\hat{f} - z\hat{I}$, $z \in \mathbb{C}$, and of its inverse $(\hat{f} - z\hat{I})^{-1}$. In what follows, for the sake of brevity, we let $\hat{f}(z)$ denote the operator $\hat{f} - z\hat{I}$,

$$\hat{f}(z) = \hat{f} - z\hat{I} = \hat{f} - z\hat{I}_{D_f},$$

and conventionally let the operator $\hat{\mathcal{R}}(z)$ denote its inverse $(\hat{f} - z\hat{I})^{-1}$,

$$\hat{\mathcal{R}}(z) = (\hat{f} - z\hat{I})^{-1} = \hat{f}(z)^{-1}.$$

For the closure $\overline{\hat{f}}$ of a closable operator $\hat{f}$, we use the natural notation $\overline{\hat{f}}(z) = \overline{\hat{f}} - z\hat{I}$ and $\overline{\hat{\mathcal{R}}}(z) = (\overline{\hat{f}}(z))^{-1} = (\overline{\hat{f}} - z\hat{I})^{-1}$.

In the finite-dimensional case in which all operators are bounded and are conventionally defined everywhere, by the spectrum of an operator $\hat{f}$ is meant the set of its eigenvalues, i.e., the set of numbers $\lambda \in \mathbb{C}$ for which $\ker \hat{f}(\lambda) \neq \{0\}$ and the operator $\hat{\mathcal{R}}(\lambda)$ does not exist.

Other points of the complex plane, usually denoted by z, are called regular points. For a regular point z, the operator $\hat{\mathcal{R}}(z)$ exists and is bounded and defined everywhere; the latter implies that the equation $\hat{f}(z)\xi = \eta$ is uniquely resolvable for any η: $\xi = \hat{\mathcal{R}}(z)\,\eta$.

In the infinite-dimensional case, there is another possibility: the operator $\hat{\mathcal{R}}(z)$ exists, but it is unbounded or it is bounded but not densely defined.

We note that for a closed $\hat{f}$, the last case will allow a more precise formulation after a preliminary simple lemma.

Lemma 2.32. *Let $\hat{f}$ be a closed operator, let the operator $\hat{f}(z)$ be invertible, and let its inverse $\hat{\mathcal{R}}(z)$ be bounded. Then the range $R_{f(z)}$ of the operator $\hat{f}(z)$, which is the domain $D_{\mathcal{R}(z)}$ of the inverse $\hat{\mathcal{R}}(z)$, is closed, $R_{f(z)} = D_{\mathcal{R}(z)} = \overline{D_{\mathcal{R}(z)}} = \overline{R_{f(z)}}$, i.e., $R_{f(z)} = D_{\mathcal{R}(z)}$ is either a closed subspace in $\mathfrak{H}$ or is the whole of $\mathfrak{H}$.*

After the remark that for a closed $\hat{f}$, the operator $\hat{f} - z\hat{I}$ is also closed, see (2.19), the assertion of the lemma becomes a paraphrase of Lemma 2.29.[17]

The case that the operator $\hat{\mathcal{R}}(z)$ is bounded but is not densely defined now can be formulated for a closed $\hat{f}$ as "the operator $\hat{\mathcal{R}}(z)$ exists, is bounded, but is defined on a closed subspace in $\mathfrak{H}$."

We now give a definition of the spectrum of an operator $\hat{f}$ in a Hilbert space in two steps.

Definition 2.33. A number $z \in \mathbb{C}$ is called a *regular point* or a point of the *resolvent set* of an operator $\hat{f}$ if the operator $\hat{f}(z)$ is invertible and the inverse operator $\hat{\mathcal{R}}(z)$ is bounded and densely defined. For a closed $\hat{f}$, the last condition is replaced by "defined everywhere, or $R_{f(z)} = \mathfrak{H}$" by virtue of Lemma 2.32.

We let $\operatorname{regp} \hat{f}$ denote the resolvent set of an operator $\hat{f}$.

The operator-valued function $\hat{\mathcal{R}}(z)$ of a complex variable z defined on the resolvent set, i.e., for $z \in \operatorname{regp} \hat{f}$, is called the *resolvent of an operator* $\hat{f}$. Sometimes, the operator $\hat{\mathcal{R}}(z)$ with a fixed $z \in \operatorname{regp} \hat{f}$ is also referred to as the resolvent (at the point z).

[17] We separate Lemmas 2.32 and 2.29 for our later convenience.

For any $z \in \operatorname{regp} \hat{f}$, the domain and the range of the resolvent of a closed operator $\hat{f}$ are respectively $\mathfrak{H}$ and D_f. This implies that the equation $\hat{f}(z)\,\xi = \eta$ is uniquely resolvable with respect to ξ belonging to D_f for any $\eta \in \mathfrak{H}$: $\xi = \hat{\mathcal{R}}(z)\,\eta$ (whence the name resolvent), which is equivalent to the equalities $\hat{f}(z)\,\hat{\mathcal{R}}(z) = \hat{I}$, $\hat{\mathcal{R}}(z)\,\hat{f}(z) = \hat{I}_{D_f}$. In particular, we have

$$\hat{\mathcal{R}}(z') = \hat{\mathcal{R}}(z')\,\hat{f}(z)\,\hat{\mathcal{R}}(z)\,,\ \hat{\mathcal{R}}(z) = \hat{\mathcal{R}}(z')\,\hat{f}(z')\,\hat{\mathcal{R}}(z)\,,\ \forall z, z' \in \operatorname{regp} \hat{f}\,. \tag{2.21}$$

Definition 2.34. The complement of the resolvent set in the complex plane $\mathbb{C}$ is called the *spectrum of an operator* $\hat{f}$ and is denoted by $\operatorname{spec} \hat{f}$, so that

$$\operatorname{regp} \hat{f} \cup \operatorname{spec} \hat{f} = \mathbb{C},\ \ \operatorname{regp} \hat{f} \cap \operatorname{spec} \hat{f} = \emptyset.$$

The points of the spectrum are usually denoted by λ. It is evident that the eigenvalues of an operator $\hat{f}$ belongs to its spectrum, but in general, they do not exhaust it. The eigenvalues form the *point spectrum*; if λ belongs to the point spectrum, the operator $\hat{\mathcal{R}}(\lambda)$ does not exist. For s.a. operators, a more detailed specification of the spectrum is given in Sect. 2.8.6.

Lemma 2.35. *(1) The resolvent sets of a closable operator $\hat{f}$ and of its closure $\overline{\hat{f}}$ are the same,* $\operatorname{regp} \hat{f} = \operatorname{regp} \overline{\hat{f}}$. *Therefore, their spectra coincide,* $\operatorname{spec} \hat{f} = \operatorname{spec} \overline{\hat{f}}$.

(2) The resolvent set $\operatorname{regp} \hat{f}$ *of a closable operator $\hat{f}$ is an open set in $\mathbb{C}$, and therefore, its spectrum* $\operatorname{spec} \hat{f}$ *is a closed set.*[18]

Proof. (1) An operator $\hat{f}(z)$ is closable together with $\hat{f}$, and $\overline{\hat{f}(z)} = \overline{\hat{f}}(z)$; see (2.19). Then by Lemma 2.28, the equality $(\overline{\hat{f}}(z))^{-1} = \overline{(\hat{f}(z)^{-1})}$, or $\hat{\overline{\mathcal{R}}}(z) = \overline{\hat{\mathcal{R}}(z)}$, holds if one of its sides has a sense. It immediately follows that for a closable operator $\hat{f}$, a number $z \in \mathbb{C}$ is a regular point of $\hat{f}$ iff z is a regular point of its closure $\overline{\hat{f}}$.

Necessity: Let z be a regular point of $\hat{f}$. Then the bounded operator $\hat{\mathcal{R}}(z)$ has a bounded closure $\overline{\hat{\mathcal{R}}(z)} = \hat{\overline{\mathcal{R}}}(z)$ with the domain $D_{\overline{\hat{\mathcal{R}}(z)}} = \overline{D_{\hat{\mathcal{R}}(z)}} = \mathfrak{H} = D_{\hat{\overline{\mathcal{R}}}(z)}$. Sufficiency is evident.

(2) In view of item (1), it suffices to consider a closed operator $\hat{f}$. Let $z \in \operatorname{regp} \hat{f}$. Then the operator $\hat{f}(z + \delta z)$ defined on D_f, as well as $\hat{f}(z)$, allows the representation

$$\hat{f}(z + \delta z) = \hat{f}(z) - \delta z \hat{I}_{D_f} = \hat{f}(z) - \delta z \hat{\mathcal{R}}(z)\,\hat{f}(z) = (\hat{I} - \delta z \hat{\mathcal{R}}(z))\,\hat{f}(z)\,.$$

[18] In fact, the spectrum of any operator is closed [125].

If $|\delta z| \left\| \hat{\mathcal{R}}(z) \right\| < 1$, the operator $\delta z \hat{\mathcal{R}}(z)$ satisfies the conditions of Lemma 2.31, and therefore, the operator $(\hat{I} - \delta z \hat{\mathcal{R}}(z))^{-1}$ exists and is bounded and defined everywhere as well as $\hat{\mathcal{R}}(z)$. Then by virtue of Lemma 2.30, the operator $\hat{f}(z+\delta z)$ is invertible, and its inverse is given by $\hat{\mathcal{R}}(z+\delta z) = \hat{\mathcal{R}}(z)\,(\hat{I} - \delta z \hat{\mathcal{R}}(z))^{-1}$. In addition, $\hat{\mathcal{R}}(z+\delta z)$ is bounded and defined everywhere as the product of bounded operators defined everywhere, which means that the point $z + \delta z$ also belongs to regp $\hat{f}$. We thus obtain that an ε-neighborhood of a regular point z with $\varepsilon < \|\hat{\mathcal{R}}(z)\|^{-1}$ is a set of regular points, which completes the proof of the lemma.

For a closed operator $\hat{f}$ and arbitrary $z,z' \in$ regp $\hat{f}$, we have the Hilbert identity

$$\hat{\mathcal{R}}\left(z'\right) - \hat{\mathcal{R}}(z) = \left(z' - z\right)\hat{\mathcal{R}}\left(z'\right)\hat{\mathcal{R}}(z)\,.$$

To prove this identity, it is sufficient to use in sequence the identity

$$\hat{\mathcal{R}}\left(z'\right) - \hat{\mathcal{R}}(z) = \hat{\mathcal{R}}\left(z'\right)\hat{f}(z)\,\hat{\mathcal{R}}(z) - \hat{\mathcal{R}}\left(z'\right)\hat{f}\left(z'\right)\hat{\mathcal{R}}(z)$$

following from (2.21), (2.16), and (2.17), taking into account that $D_{\mathcal{R}(z')} = \mathfrak{H}$. It follows from the Hilbert identity that for arbitrary regular points z and z', the respective resolvents $\hat{\mathcal{R}}(z)$ and $\hat{\mathcal{R}}(z')$ commute with each other, $[\hat{\mathcal{R}}(z), \hat{\mathcal{R}}(z')] = 0$, and that the resolvent is an analytic function on the resolvent set (in the sense of uniform operator topology) with derivative $d\hat{\mathcal{R}}(z)/dz = \hat{\mathcal{R}}^2(z)$.

If $\hat{f}$ is a bounded operator defined everywhere, then a point z such that $|z| > \|\hat{f}\|$ is a regular point of $\hat{f}$, and therefore, the spectrum of $\hat{f}$ lies within the circle of radius $\|\hat{f}\|$, spec $\hat{f} \subseteq \{z : |z| \leq \|\hat{f}\|\}$. To prove this assertion, it is sufficient to use the representation $\hat{f}(z) = -z(\hat{I} - z^{-1}\hat{f})$ and then Lemma 2.31. □

2.6 Adjoint Operators

2.6.1 Definition and Properties

By analogy with an inverse operator, an adjoint operator is defined in the language of graphs simply via the replacement of the unitary operator Σ_1 in $\mathbb{H}$ by the unitary operator $\mathcal{E}$ defined by (2.14). But the construction is more involved.

Let $\mathbb{G}_f = \{(\xi / \hat{f}\xi)\} \subset \mathbb{H}$ be a graph of an operator $\hat{f}$. We consider a subspace $\mathcal{E}\mathbb{G}_f = \{(\hat{f}\xi / -\xi)\} \subset \mathbb{H}$. In connection with the decomposition

$$\mathbb{H} = \mathfrak{H} \oplus \mathfrak{H} = \overline{\mathcal{E}\mathbb{G}_f} \oplus \left(\mathcal{E}\mathbb{G}_f\right)^{\perp},$$

the question arises whether the orthogonal complement $\left(\mathcal{E}\mathbb{G}_f\right)^{\perp}$ of the subspace $\mathcal{E}\mathbb{G}_f$ is a graph.[19] By definition, the subspace $\left(\mathcal{E}\mathbb{G}_f\right)^{\perp}$ is given by

$$\left(\mathcal{E}\mathbb{G}_f\right)^{\perp} = \left\{(\xi_* \diagup \eta) \in \mathbb{H} : \left(\xi_*, \hat{f}\xi\right) - (\eta, \xi) = 0,\ \forall \xi \in D_f\right\}. \tag{2.22}$$

Definition 2.36. Let $\left(\mathcal{E}\mathbb{G}_f\right)^{\perp}$ be a graph and therefore determine an operator. This operator is called the *adjoint operator*, or simply the adjoint, of $\hat{f}$ and is denoted by $\hat{f}^+$ such that $\eta = \hat{f}^+\xi_*$,

$$\mathbb{G}_{f^+} = \left\{\left(\xi_* \diagup \eta = \hat{f}^+\xi_*\right)\right\} = \left(\mathcal{E}\mathbb{G}_f\right)^{\perp}. \tag{2.23}$$

The graph criterion (2.11), Lemma 2.19, provides a criterion for the existence of the adjoint $\hat{f}^+$ of an operator $\hat{f}$: the operator $\hat{f}^+$ exists iff $\hat{f}$ is densely defined, $\overline{D_f} = \mathfrak{H}$. Indeed, (2.22) and (2.11) yield the following chain of conclusions: $\xi_* = 0 \Longrightarrow (\eta, \xi) = 0,\ \forall \xi \in D_f \Longrightarrow \eta = 0$ iff D_f is dense in $\mathfrak{H}$. So only a densely defined operator has an adjoint operator.

An equivalent definition of $\hat{f}^+$ in the language of maps is lengthier and goes as follows.

Definition 2.37. Given an operator $\hat{f}$, we consider the linear equation

$$\left(\xi_*, \hat{f}\xi\right) = (\eta, \xi)\,,\ \forall \xi \in D_f, \tag{2.24}$$

for pairs of vectors ξ_*, η. A vector η in each pair is uniquely determined by vector ξ_* iff the operator $\hat{f}$ is densely defined, $\overline{D_f} = \mathfrak{H}$. If so, the operator $\hat{f}$ has the adjoint operator $\hat{f}^+$, its domain is the subspace of all those vectors ξ_* for which there exist vectors η satisfying (2.24), and $\eta = \hat{f}^+\xi_*$.

We call (2.24) with a densely defined operator $\hat{f}$ the *defining equation for the adjoint operator* $\hat{f}^+$. This is the equation for the pairs of vectors ξ_* and $\eta = \hat{f}^+\xi_*$ that form respectively the domain and range of the operator $\hat{f}^+$.

We call the operation $^+$ that assigns the adjoint operator $\hat{f}^+$ to any densely defined operator $\hat{f}$, $\hat{f} \xrightarrow{+} \hat{f}^+$, *the adjoint operation*. Another name is the Hermitian adjoint operation.

[19]We can also ask whether the subspace $\mathcal{E}\mathbb{G}_f$ is a graph. In fact, we already know the answer: it is easy to see that $\mathcal{E}\mathbb{G}_f$ is a graph iff $\hat{f}$ is invertible, and if so, $\mathcal{E}\mathbb{G}_f$ determines the operator $-\hat{f}^{-1}$, $\mathcal{E}\mathbb{G}_f = \mathbb{G}_{-f^{-1}}$.

Remark 2.38. In some textbooks for physicists, the adjoint $\hat{f}^+$ is defined via its matrix elements with respect to an orthonormal basis $\{e_k\}_1^\infty$ by

$$f_{kl}^+ = \left(e_k, \hat{f}^+ e_l\right) = \left(\hat{f} e_k, e_l\right) = \overline{\left(e_l, \hat{f} e_k\right)} = \overline{f_{lk}} \,.$$

This definition is very restrictive and is generally incorrect. In general, the matrix of an operator does not determine the operator. In addition, this formulation assumes that $\{e_k\}_1^\infty \subset D_{f^+}$, and therefore that $\hat{f}^+$ is densely defined, $\overline{D_{f^+}} = \mathfrak{H}$, which is generally not the case. Finally, it follows that $(\hat{f}^+)^+ = \hat{f}$, which is generally not true. In other words, it is believed that any operator $\hat{f}$ can always be rearranged to the left in a matrix element $(\xi_*, \hat{f}\xi)$ with a cross over it: $(\xi_*, \hat{f}\xi) = (\hat{f}^+\xi_*, \xi)$, with the domain D_{f^+} not specified in any way. Strictly speaking, this definition is applicable to bounded operators defined everywhere (see below). The point of this remark is that for a given densely defined operator $\hat{f}$, and only for such an operator, the adjoint operator $\hat{f}^+$ is evaluated by solving the defining equation (2.24) for pairs ξ_* and $\eta = \hat{f}^+\xi_*$.

As an illustration, we evaluate the adjoints of some operators.

It is easy to see that $(z\hat{I})^+ = \overline{z}\hat{I}$. A simple evaluation shows that the adjoint $\hat{U}^+$ of a unitary operator $\hat{U}$ coincides with its inverse $\hat{U}^{-1}, \hat{U}^+ = \hat{U}^{-1}$, and a unitary operator $\hat{U}$ can be defined as an operator satisfying the equalities $\hat{U}^+\hat{U} = \hat{U}\hat{U}^+ = \hat{I}$.

An interesting example is presented by the above operator (2.18). The defining equation

$$\sqrt{\pi/2}\psi\,(0)\,(\xi_*, e_1) = (\eta, \psi)\,,\; e_1\,(x) = \sqrt{2/\pi}\,\sin x,\;\; \forall \text{ continuous } \psi\,(x)\,,$$

for the adjoint $\hat{f}^+$ has the following solution: Let $\psi \in \mathcal{D}\,(0, \pi)$. Because $\psi\,(0) = 0$, we find $(\eta, \psi) = 0$, $\forall \psi \in \mathcal{D}\,(0, \pi)$. Then it follows from Lemma 2.4 and Theorem 2.6 that $\eta = 0$. Taking now ψ such that $\psi\,(0) \neq 0$, we find $(\xi_*, e_1) = 0$, which implies that $D_{f^+} = \{ae_1\,(x)\,,\; \forall a \in \mathbb{C}\}^\perp$, the subspace orthogonal to $\sin x$, and $\hat{f}^+ = 0$. It is remarkable that $\hat{f}^+$ is not densely defined, and therefore, $(\hat{f}^+)^+$ does not exist. The reason is the nonclosability of $\hat{f}$ (see below).

The Riesz theorem, Theorem 2.16, provides a criterion for a vector ξ_* to belong to the domain D_{f^+} of the adjoint $\hat{f}^+$ of a densely defined operator $\hat{f}$, namely, $\xi_* \in D_{f^+}$, i.e., there exists a vector η satisfying the defining equation (2.24), iff a linear functional $\Phi_{\xi_*}(\xi) = (\xi_*, \hat{f}\xi)$, $\forall \xi \in D_f$, is bounded (continuous). The necessity is obvious: $\Phi_{\xi_*}(\xi) = (\eta, \xi)$ implies $\left|\Phi_{\xi_*}(\xi)\right| \leq \|\eta\|\;\|\xi\|$. The sufficiency is also easy to prove: the bounded functional Φ_{ξ_*} defined on the dense domain D_f is extended to the whole of $\mathfrak{H}$ by continuity as a bounded functional with the same norm, and then by Theorem 2.16, it is represented as $\Phi_{\xi_*}(\xi) = (\eta, \xi)$ with a uniquely defined η. The pair ξ_*, η is clearly a solution of the defining equation, and $\eta = \hat{f}^+\xi$.

An immediate consequence is the following lemma for bounded operators.

Lemma 2.39. *If an operator $\hat{f}$ is defined everywhere, $D_f = \mathfrak{H}$, and bounded, $\|\hat{f}\| < \infty$, then its adjoint $\hat{f}^+$ exists and is defined everywhere, $D_{f^+} = \mathfrak{H}$; it is bounded with $\|\hat{f}^+\| = \|\hat{f}\|$; and $(\hat{f}^+)^+ = \hat{f}$.*

Proof. The first assertion is evident. The second assertion follows from the estimate

$$\left|\left(\xi_*, \hat{f}\xi\right)\right| \leq \|f\| \, \|\xi_*\| \, \|\xi\| \,, \; \forall \xi, \xi_* \in \mathfrak{H} \,,$$

and from the Riesz theorem. The third assertion follows from the chain of equalities

$$\left\|\hat{f}^+\right\| = \sup_{\forall \xi, \xi_* \neq 0} \left|\left(\xi^{\mathrm{n}}, \hat{f}^+ \xi_*^{\mathrm{n}}\right)\right| = \sup_{\forall \xi, \xi_* \neq 0} \left|\left(\xi_*^{\mathrm{n}}, \hat{f}\xi^{\mathrm{n}}\right)\right| = \left\|\hat{f}\right\| \,,$$

where $\xi^{\mathrm{n}} = \xi \big/ \|\xi\|$, $\xi_*^{\mathrm{n}} = \xi_* \big/ \|\xi_*\|$. The fourth assertion follows from the evident symmetry between $\hat{f}$ and $\hat{f}^{\,+}$ in the defining equation (it is sufficient to perform complex conjugation and transposition of the left-hand side and the right-hand side in the defining equation to obtain $(\xi, \hat{f}^+\xi_*) = (\hat{f}\xi, \xi_*)$, $\forall \xi, \xi_* \in \mathfrak{H}$. □

This result is sometimes cited in textbooks on QM for physicists as a general one and is implicitly applied to unbounded operators, which is incorrect.

We cite separately the properties of adjoint operators that concern their relation to the notions of extension, invertibility, closability, and algebra.

2.6.2 Adjoint and Extensions

Lemma 2.40. *Let a densely defined operator $\hat{f}$ with the adjoint $\hat{f}^+$ have an extension $\hat{g}$, $\hat{f} \subseteq \hat{g}$. Then $\hat{g}$ has the adjoint $\hat{g}^+$, which is a restriction of $\hat{f}^+$, $\hat{g}^+ \subseteq \hat{f}^+$.*

So, extending a densely defined operator $\hat{f}$ is accompanied by restricting its adjoint $\hat{f}^+$. This fact is fundamental in what follows.

In the language of graphs, the proof is very simple (see (2.3)):

$$\mathbb{G}_f \subseteq \mathbb{G}_g \Longrightarrow \mathcal{E}\mathbb{G}_f \subseteq \mathcal{E}\mathbb{G}_g \Longrightarrow \mathbb{G}_{f^+} = (\mathcal{E}\mathbb{G}_f)^{\perp} \supseteq (\mathcal{E}\mathbb{G}_g)^{\perp} = \mathbb{G}_{g^+} \,,$$

which means that $\hat{g}^+$ exists and $\hat{g}^+ \subseteq \hat{f}^+$: the left-hand side of the last inclusion is a graph, the graph of $\hat{f}^+$. Therefore, the right-hand side is also a graph, the graph of $\hat{g}^+$, and the inclusion itself means that $\hat{g}^+ \subseteq \hat{f}^+$.

Remark 2.41. This property is useful for analyzing extensions and evaluating adjoints. Namely, let a densely defined operator $\hat{f}$ allow a restriction $\hat{f}_0$ that is also densely defined, $\overline{D_{f_0}} = \mathfrak{H}$. Let the adjoint $\hat{f}_0^+$ be easily evaluated. We then know "the rule of acting" for the adjoint $\hat{f}^+ \subseteq \hat{f}_0^+$, and it remains to find its domain D_{f+}. The domain is determined by solving the linear equation

$$\left(\xi_*, \hat{f}\xi\right) = \left(\hat{f}_0^+\xi_*, \xi\right), \ \forall \xi \in D_f \ , \ \text{for } \xi_* \in D_{f+} \subseteq D_{f_0^+} \ ,$$

to which the defining equation for $\hat{f}^+$ reduces after taking the equality $\hat{f}^+\xi_* = \hat{f}_0^+\xi_*, \forall \xi_* \in D_{f+}$, into account. This method is often used for differential operators. In particular, for differential operators with smooth coefficients in an interval (a, b) of the real axis, the set $\mathcal{D}(a, b)$ of compactly supported smooth functions is taken as D_{f_0}. Then the methods of distribution theory [88] are used for evaluating $\hat{f}_0^+$, while the adjoints $\hat{f}^+$ of different extensions $\hat{f}$ of $\hat{f}_0$ are naturally specified by boundary conditions for functions belonging to $D_{f_0^+}$ (see Chap. 4).

2.6.3 Adjoint, Closability, and Closure

Lemma 2.42. *An adjoint operator is closed, $\hat{f}^+ = \overline{\hat{f}^+}$ (although the operator $\hat{f}$ can be nonclosed and even nonclosable). The adjoint of a closable densely defined operator $\hat{f}$ and the adjoint of its closure $\overline{\hat{f}}$ are identical, $\hat{f}^+ = \overline{\hat{f}^+} = (\overline{\hat{f}})^+$(the adjoint operation $^+$ and the closure operation $^-$ commute if they make sense).*

Proof. The proof reduces to chains of graph equalities. For any densely defined operator $\hat{f}$, the chain of equalities

$$\mathbb{G}_{f+} = (\mathcal{E}\mathbb{G}_f)^\perp = \overline{(\mathcal{E}\mathbb{G}_f)^\perp} = \mathbb{G}_{\overline{f+}}$$

holds, while for a closable densely defined operator $\hat{f}$, the equalities can be continued to

$$\overline{(\mathcal{E}\mathbb{G}_f)^\perp} = \left(\overline{\mathcal{E}\mathbb{G}_f}\right)^\perp = (\mathcal{E}\overline{\mathbb{G}_f})^\perp = (\mathcal{E}\mathbb{G}_{\overline{f}})^\perp = \mathbb{G}_{\overline{f}^+},$$

where we successively use (2.2) and (2.12). □

The following lemma is of great importance.

Lemma 2.43. *A densely defined operator $\hat{f}$ is closable iff its adjoint $\hat{f}^+$ is densely defined or, which is the same, the operator $(\hat{f}^+)^+$exists. For any closable densely defined operator $\hat{f}$, we have $(\hat{f}^+)^+ = \overline{\hat{f}}$ (the double adjoint operation is equivalent to the closure operation); in particular, if $\hat{f}$ is densely defined and closed, then $(\hat{f}^+)^+ = \hat{f}$.*

Proof. The proof reduces to a chain of graph equalities, which can be read from left to right and from right to left:

$$\mathbb{G}_{(f^+)^+} = \left(\mathcal{E}\mathbb{G}_{f^+}\right)^{\perp} = \mathcal{E}\left(\left(\mathcal{E}\mathbb{G}_f\right)^{\perp}\right)^{\perp} = \mathcal{E}\left(\overline{\mathcal{E}\mathbb{G}_f}\right) = (\mathcal{E})^2\,\overline{\mathbb{G}_f} = \overline{\mathbb{G}_f} = \mathbb{G}_{\overline{f}},$$

where we use sequentially (2.13), (2.6), (2.12), the equality $(\mathcal{E})^2 = -\widehat{\mathbb{I}}$, where $\widehat{\mathbb{I}}$ is the identity operator in $\mathbb{H}$, and the fact that a multiple of unity transforms any subspace to the same subspace. □

Lemma 2.43 yields not only a criterion for closability of a densely defined operator $\hat{f}$ (for a counterexample, see operator (2.18)), but also a method for constructing its closure $\overline{\hat{f}}$. This method is effectively used in the theory of differential operators; see Chap. 4.

Lemmas 2.39, 2.40, and 2.42 together with Lemma 2.23 and Theorem 2.17 allow us to prove an important theorem.

Theorem 2.44. *A closed operator $\hat{f}$, $\hat{f} = \overline{\hat{f}}$, defined everywhere, $D_f = \mathfrak{H}$, is bounded, $\|\hat{f}\| < \infty$.*

Proof. The idea of the proof is to show that the adjoint $\hat{f}^+$ of $\hat{f}$ is bounded and defined everywhere. Let $\{\xi_*^{\mathrm{n}}\}$ be the set of all unit vectors in D_{f^+},

$$\{\xi_*^{\mathrm{n}}\} = \left\{\xi_*^{\mathrm{n}} : \xi_*^{\mathrm{n}} \in D_{f^+},\ \|\xi_*^{\mathrm{n}}\| = 1\right\}.$$

Because $D_f = \mathfrak{H}$ and $\xi_*^{\mathrm{n}} \in D_{f^+}$, we have

$$\left(\xi_*^{\mathrm{n}}, \hat{f}\xi\right) = \left(\hat{f}^+\xi_*^{\mathrm{n}}, \xi\right) = \overline{\left(\xi, \hat{f}^+\xi_*^{\mathrm{n}}\right)},\ \forall\xi \in \mathfrak{H},\ \forall\xi_*^{\mathrm{n}}.$$

By the Cauchy–Schwarz inequality, it follows that

$$\left|\left(\xi, \hat{f}^+\xi_*^{\mathrm{n}}\right)\right| = \left|\left(\xi_*^{\mathrm{n}}, \hat{f}\xi\right)\right| \le \left\|\hat{f}\xi\right\|,\ \forall\xi \in \mathfrak{H},\ \forall\xi_*^{\mathrm{n}},$$

which means that the set $\{\hat{f}^+\xi_*^{\mathrm{n}}\}$ is weakly bounded. By Theorem 2.17, the set $\{\hat{f}^+\xi_*^{\mathrm{n}}\}$ is then strongly bounded, i.e., $\|\hat{f}^+\xi_*^{\mathrm{n}}\| \le C$, $\forall\xi_*^{\mathrm{n}}$, which implies that $\|\hat{f}^+\| \le \infty$, i.e., the operator $\hat{f}^+$ is bounded. By Lemma 2.42, $\hat{f}^+$ is closed; hence by Lemma 2.23, its domain is a closed subspace, $D_{f^+} = \overline{D_{f^+}}$. But by Lemma 2.43 as applied to the operator $\hat{f}$, we have $\overline{D_{f^+}} = \mathfrak{H}$, which yields $D_{f^+} = \mathfrak{H}$, and $\hat{f} = (\hat{f}^+)^+$. The operator $\hat{f}^+$ is thus bounded and defined everywhere. Applying now Lemma 2.39 to the operator $\hat{f}^+$ and using the equality $\hat{f} = (\hat{f}^+)^+$, we finally obtain that the initial operator $\hat{f}$ is bounded. □

This theorem is very important for QM. Unbounded closed operators, in particular unbounded s.a. operators, cannot be defined everywhere in the whole of $\mathfrak{H}$. Therefore, we must be careful in finding an appropriate domain for any unbounded QM observable to ensure its self-adjointness. A direct consequence of Theorem 2.44 is the following useful lemma concerning the spectrum of a closed operator.

Lemma 2.45. *A number $z \in \mathbb{C}$ is a regular point of a closed operator $\hat{f}$ iff the operator $\hat{f}(z) = \hat{f} - z\hat{I}$ is invertible and the inverse operator $\hat{R}(z)$ is defined everywhere, or $R_{f(z)} = \mathfrak{H}$. In fact, this is a reduced definition of a regular point for a closed operator.*

Proof. Necessity is evident by the definition of a regular point; see Sect. 2.6.3.

Sufficiency. Let $\hat{f}(z)$ be invertible, and let $R_{f(z)} = \mathfrak{H}$. Because $\hat{f}(z)$ is closed as well as $\hat{f}$, its inverse $\hat{R}(z)$ defined everywhere is also closed; see Lemma 2.29. Then by the theorem, $\hat{R}(z)$ is bounded, and therefore, z is a regular point of $\hat{f}$ by the same definition. □

2.6.4 Adjoint and Invertibility

We first prove a lemma.

Lemma 2.46. *For a densely defined operator $\hat{f}$, the orthogonal complement of its range is the kernel of its adjoint, $\left(R_f\right)^{\perp} = \ker \hat{f}^{+}$, so that the decomposition $\mathfrak{H} = \overline{R_f} \oplus \ker \hat{f}^{+}$ holds. If, in addition, the operator $\hat{f}$ is closable, $\hat{f} \subseteq \overline{\hat{f}}$, then we also have $\ker \overline{\hat{f}} = \overline{R_{f^+}}$, so that the decomposition $\mathfrak{H} = \overline{R_{f^+}} \oplus \ker \overline{\hat{f}}$ holds.*

Proof. For $\xi_* \in \ker \hat{f}^{+}$, the defining equation (2.24) becomes $(\xi_*, \hat{f}\xi) = 0$, $\forall \xi \in D_f$, which means that $\xi_* \in \left(R_f\right)^{\perp}$, and conversely, if $\xi_* \in \left(R_f\right)^{\perp}$, we have $(\xi_*, \hat{f}\xi) = 0 = (0, \xi)$, $\forall \xi \in D_f$, which implies that $\xi_* \in D_{f^+}$ and $\hat{f}^{+}\xi_* = 0$, i.e., $\xi_* \in \ker \hat{f}^{+}$. It remains to refer to (2.4) to prove the first assertion of the lemma. If, in addition, $\hat{f} \subseteq \overline{\hat{f}}$, then by Lemma 2.43, the adjoint $\hat{f}^{+}$ is densely defined and $(\hat{f}^{+})^{+} = \overline{\hat{f}}$, and it remains to apply the first assertion to the operator $\hat{f}^{+}$ to complete the proof. □

Corollary 2.47. *The adjoint of a densely defined operator $\hat{f}$ is invertible,* $\ker \hat{f}^{+} = 0$, *iff the range of $\hat{f}$ is dense in $\mathfrak{H}$, $\overline{R_f} = \mathfrak{H}$. If, in addition, the operator $\hat{f}$ is closable, then its closure $\overline{\hat{f}}$ is invertible, together with $\hat{f}$,* $\ker \overline{\hat{f}} = \ker \hat{f} = 0$, *iff $\overline{R_{f^+}} = \mathfrak{H}$.*

It is interesting to compare the operators$(\hat{f}^{+})^{-1}$ and $(\hat{f}^{-1})^{+}$. It may be that one of these operators exists, whereas the other does not, for example, if $\overline{D_f} = \mathfrak{H}$ and $\ker \hat{f}^{+} = 0$, but $\ker \hat{f} \neq \{0\}$, or $\ker \hat{f} = \{0\}$ and $\overline{D_{f^{-1}}} = \mathfrak{H}$, but $\overline{D_f} \neq \mathfrak{H}$, etc. But if both operators exist simultaneously, they are identical.

Lemma 2.48. *The operators* $(\hat{f}^{-1})^+$ *and* $(\hat{f}^+)^{-1}$ *exist simultaneously iff* $\overline{D_f} = \mathfrak{H}$ *and* $\ker \hat{f} = \ker \hat{f}^+ = \{0\}$ *(for a closed operator,* $\hat{f} = \overline{\hat{f}}$*, this is equivalent to the equalities* $\overline{D_f} = \overline{R_f} = \overline{R_{f+}} = \mathfrak{H}$*), and if so, the equality* $(\hat{f}^{-1})^+ = (\hat{f}^+)^{-1}$*holds (the inversion operation* $^{-1}$ *and the adjoint operation* $^+$ *commute if they make sense).*

Proof. The proof of the first assertion reduces to the reference to the criteria for invertibility and the existence of the adjoint and to Lemma 2.46. The proof of the second assertion reduces to the chain of graph equalities

$$\begin{aligned}\mathbb{G}_{(f^{-1})^+} &= \left(\mathcal{E}\left(\Sigma_1\mathbb{G}_f\right)\right)^\perp = \left(-\Sigma_1\mathcal{E}\mathbb{G}_f\right)^\perp = -\Sigma_1\left(\mathcal{E}\mathbb{G}_f\right)^\perp \\ &= \Sigma_1\mathbb{G}_{f+} = \mathbb{G}_{(f+)^{-1}}\,,\end{aligned}$$

where we use the equalities $\mathcal{E}\Sigma_1 = -\Sigma_1\mathcal{E}$ and (2.13). □

2.6.5 *Adjoint Operation and Algebra*

With the adjoint operation $^+$, the algebra of bounded operators defined everywhere becomes a normed associative algebra with involution:

$$\left(a\hat{f}\right)^+ = \overline{a}\hat{f}^+,\ \forall a \in \mathbb{C}\,;\ \left(\hat{f}+\hat{g}\right)^+ = \hat{f}^+ + \hat{g}^+;\ \left(\hat{f}\hat{g}\right)^+ = \hat{g}^+\hat{f}^+\,, \tag{2.25}$$

and with the equality $\|\hat{f}\| = \|\hat{f}^+\|$. Such an algebra is called a C^*-algebra.

Some textbooks on QM for physicists implicitly extend the above rules for bounded operators to unbounded ones, which is incorrect.

For unbounded densely defined operators, (2.25) are modified as follows:

(a) $(a\hat{f})^+ = \overline{a}\hat{f}^+$.

(b) If the sum $\hat{f} + \hat{g}$ is densely defined, then its adjoint $(\hat{f}+\hat{g})^+$exists, and we have
$$\left(\hat{f}+\hat{g}\right)^+ \supseteq \hat{f}^+ + \hat{g}^+,\ \text{if}\ \overline{D_f \cap D_g} = \mathfrak{H}.$$

(c) If one of the operators is bounded and defined everywhere, the inclusion becomes an equality:
$$\left(\hat{f}+\hat{g}\right)^+ = \hat{f}^+ + \hat{g}^+,\ \text{if}\ D_f = \mathfrak{H}, \text{or}\ D_g = \mathfrak{H}\,,$$
in particular,
$$\left(\hat{f}\left(z\right)\right)^+ = \hat{f}^+ - \overline{z}\hat{I} = \hat{f}^+(\overline{z}). \tag{2.26}$$

(d) If the product $\hat{f}\hat{g}$ is densely defined, then its adjoint exists and we have

$$\left(\hat{f}\hat{g}\right)^{+} \supseteq \hat{g}^{+}\hat{f}^{+}, \text{ if } \overline{D_{fg}} = \mathfrak{H}. \tag{2.27}$$

(e) If $\hat{f}$ is bounded and defined everywhere, the inclusion becomes an equality:

$$\left(\hat{f}\hat{g}\right)^{+} = \hat{g}^{+}\hat{f}^{+}, \text{ if } D_f = \mathfrak{H}. \tag{2.28}$$

2.7 Symmetric Operators

2.7.1 Definition and Properties

Definition 2.49. A densely defined operator $\hat{f}$ is called a *symmetric operator* or *Hermitian operator* if its adjoint $\hat{f}^{+}$ is an extension of $\hat{f}$, $\hat{f} \subseteq \hat{f}^{+}$. In the language of graphs, this means that $\mathbb{G}_f \subseteq \mathbb{G}_{f+} = \left(\mathcal{E}\mathbb{G}_f\right)^{\perp}$. In the language of maps, this means that

$$\left(\eta, \hat{f}\xi\right) = \left(\hat{f}\eta, \xi\right), \ \forall \xi, \eta \in D_f . \tag{2.29}$$

We note that to prove the symmetricity, or hermiticity, of a densely defined operator $\hat{f}$, we need not know its adjoint $\hat{f}^{+}$; it is sufficient to verify (2.29).

In some textbooks on QM for physicists, this definition is considered the definition of an s.a. operator. This implicitly means that only bounded operators defined everywhere are considered (see Sect. 2.8.5 below). For unbounded operators, symmetricity and self-adjointness are different notions: self-adjointness implies symmetry, but not vice versa. Symmetricity is generally insufficient for QM observables; they must be s.a.

We cite two simple criteria for symmetricity.

Lemma 2.50. *A densely defined operator is symmetric:*

(i) iff its matrix $f_{mn} = (e_m, \hat{f}e_n)$ *with respect to an orthonormal basis* $\{e_n\}_1^{\infty} \subset D_f$ *is Hermitian,* $f_{mn} = \overline{f_{nm}}$ *(whence the name "Hermitian"), or*

(ii) iff all means of the operator are real, $(\xi, \hat{f}\xi) = \overline{\left(\xi, \hat{f}\xi\right)}$, $\forall \xi \in D_f$.

Proof. For the proof we note only that the necessity follows directly from (2.29), while the sufficiency of (i) is proved by a verification of (2.29) starting from $\xi, \eta \in L(\{e_n\}_1^{\infty})$, and then proceeding by extension to any $\xi, \eta \in D_f$ based on the continuity arguments, whereas the sufficiency of (ii) follows from the remark that

$$\left(\xi + z\eta, \hat{f}(\xi + z\eta)\right) - \left(\xi, \hat{f}\xi\right) - |z|^2 \left(\eta, \hat{f}\eta\right) = \bar{z}\left(\eta, \hat{f}\xi\right) + z\left(\xi, \hat{f}\eta\right)$$

is a real number for any $z \in \mathbb{C}$. □

We emphasize that for unbounded operators, the cited criteria are the criteria for symmetricity, but not for self-adjointness.

Corollary 2.51. *A densely defined operator bounded from above or from below is symmetric.*

Indeed, all means of such an operator are necessarily real-valued, and by criterion (ii), the operator is symmetric.

If a symmetric operator is bounded and closed, then by Lemma 2.23, it is defined everywhere. By continuity arguments, a bounded symmetric operator $\hat{f}$ with $D_f \neq \mathfrak{H}$ can be extended to a bounded symmetric operator defined everywhere (and therefore closed). For the general relation between symmetricity and closability, see below.

Lemma 2.52. *For symmetric operators, the following equalities hold ($\xi \in D_f$):*

$$\left\|\hat{f}\right\| = \sup_{\|\xi\|=1} \left\|\hat{f}\xi\right\| = \sup_{\eta;\|\xi\|,\|\eta\|=1} \left|\left(\eta, \hat{f}\xi\right)\right| = \sup_{\|\xi\|=1} \left|\left(\xi\,, \hat{f}\xi\right)\right|. \tag{2.30}$$

It follows that if a symmetric operator is bounded, $\|\hat{f}\| = c < \infty$, it is bounded from below and from above, $-c\hat{I} \leq \hat{f} \leq c\hat{I}$, and conversely, if a symmetric operator is bounded from below and from above, $-c\hat{I} \leq \hat{f} \leq b\hat{I}$, it is bounded and $\|\hat{f}\| \leq \max(|c|, |b|)$.

Strictly speaking, these equalities are meaningful for bounded operators. The meaning of the equalities for unbounded operators is that all three suprema are infinite.

Proof. The first equality is the definition (2.15) of the norm of an operator. The second equality holds for any operators because of the Cauchy–Schwarz inequality, which yields

$$\sup_{\eta;\|\xi\|,\|\eta\|=1} \left|\left(\eta, \hat{f}\xi\right)\right| \leq \sup_{\|\xi\|=1} \left\|\hat{f}\xi\right\|,$$

and because of the evident inverse inequality,

$$\sup_{\eta;\|\xi\|,\|\eta\|=1} \left|\left(\eta, \hat{f}\xi\right)\right| \geq \sup_{\|\xi\|=1,\hat{f}\xi\neq 0;\,\eta=\hat{f}\xi/\|\hat{f}\xi\|} \left|\left(\eta, \hat{f}\xi\right)\right| = \sup_{\|\xi\|=1} \left\|\hat{f}\xi\right\|.$$

The third equality is characteristic of symmetric operators. We first prove it for a bounded symmetric operator assuming, without loss of generality, that the operator is defined everywhere. The proof is based on the general equality ($\forall z \in \mathbb{C}$)

$$\bar{z}\left(\eta, \hat{f}\xi\right) + z\left(\xi, \hat{f}\eta\right) = \frac{1}{2}\left[\left(\xi + z\eta, \hat{f}(\xi + z\eta)\right) - \left(\xi - z\eta, \hat{f}(\xi - z\eta)\right)\right],$$

(one of the so-called polarization formulas) and on the equality $(\xi, \hat{f}\eta) = \overline{(\eta, \hat{f}\xi)}$ for symmetric operators. Let $(\eta, \hat{f}\xi) = |(\eta, \hat{f}\xi)|\mathrm{e}^{\mathrm{i}\varphi}$, and let $z = \mathrm{e}^{\mathrm{i}\varphi}$. Then the first equality becomes

$$\left|\left(\eta, \hat{f}\xi\right)\right| = \frac{1}{4}\left[\left(\xi + \mathrm{e}^{\mathrm{i}\varphi}\eta, \hat{f}(\xi + \mathrm{e}^{\mathrm{i}\varphi}\eta)\right) - \left(\xi - \mathrm{e}^{\mathrm{i}\varphi}\eta, \hat{f}(\xi - \mathrm{e}^{\mathrm{i}\varphi}\eta)\right)\right].$$

Based on this equality and using the intermediate notation $u = \xi + \mathrm{e}^{\mathrm{i}\varphi}\eta$, $\upsilon = \xi - \mathrm{e}^{\mathrm{i}\varphi}\eta$, we arrive at the inequality

$$\begin{aligned}\left|\left(\eta, \hat{f}\xi\right)\right| &\le \frac{1}{4}\left[\left|\left(u, \hat{f}u\right)\right| + \left|\left(\upsilon, \hat{f}\upsilon\right)\right|\right] = \frac{1}{4}\left[\left(u^{\mathrm{n}}, \hat{f}u^{\mathrm{n}}\right)\|u\|^2\right.\\ &\quad \left. + \left(\upsilon^{\mathrm{n}}, \hat{f}\upsilon^{\mathrm{n}}\right)\|\upsilon\|^2\right] \le \frac{1}{4}\sup_{\|\zeta\|=1}\left|\left(\zeta, \hat{f}\zeta\right)\right|\left(\|u\|^2 + \|\upsilon\|^2\right)\\ &= \frac{1}{2}\sup_{\|\zeta\|=1}\left|\left(\zeta, \hat{f}\zeta\right)\right|\left(\|\xi\|^2 + \|\eta\|^2\right),\ u^{\mathrm{n}} = u/\|u\|,\ \upsilon^{\mathrm{n}} = \upsilon/\|\upsilon\|,\end{aligned}$$

whence the final inequality

$$\sup_{\|\xi\|,\|\eta\|=1}\left|\left(\eta, \hat{f}\xi\right)\right| \le \sup_{\|\xi\|=1}\left|\left(\xi, \hat{f}\xi\right)\right|$$

follows. The inverse inequality is evident, which yields the required equality

$$\sup_{\|\xi\|,\|\eta\|=1}\left|\left(\eta, \hat{f}\xi\right)\right| = \sup_{\|\xi\|=1}\left|\left(\xi, \hat{f}\xi\right)\right| = \sup_{\|\xi\|=1}\left\|\hat{f}\xi\right\|.$$

For unbounded symmetric operators, which are densely defined by definition, the equality

$$\sup_{\xi\in D_f,\,\eta;\|\xi\|,\|\eta\|=1}\left|\left(\eta, \hat{f}\xi\right)\right| = \sup_{\xi,\,\eta\in D_f;\|\xi\|,\|\eta\|=1}\left|\left(\eta, \hat{f}\xi\right)\right|$$

holds because any vector $\eta \in \mathfrak{H}$ can be approximated by vectors belonging to D_f with arbitrary accuracy. The infinite value of $\sup\limits_{\xi\in D_f,\,\|\xi\|=1}|(\xi, \hat{f}\xi)|$ for unbounded symmetric operators then follows from the naturally modified above estimates (the proof is by contradiction); we leave the details to the reader. □

2.7.2 Symmetricity and Algebra

The algebraic properties of symmetric operators directly follow from the relation between the adjoint operation and algebra; see Sect. 2.6.5.

Multiplication by a real number transforms a symmetric operator into a symmetric one:

$$\hat{f} \subseteq \hat{f}^{+},\ a \in \mathbb{R} \Longrightarrow a\hat{f} \subseteq a\hat{f}^{+} = \left(a\hat{f}\right)^{+};$$

the densely defined sum of symmetric operators is a symmetric operator:

$$\hat{f} \subseteq \hat{f}^{+},\ \hat{g} \subseteq \hat{g}^{+},\ \overline{D_f \cap D_g} = \mathfrak{H} \Longrightarrow \hat{f} + \hat{g} \subseteq \hat{f}^{+} + \hat{g}^{+} \subseteq \left(\hat{f} + \hat{g}\right)^{+},$$

the last inclusion becoming an equality if one of the operators is bounded and defined everywhere, in particular,

$$\hat{f} - a\hat{I} \subseteq \hat{f}^{+} - a\hat{I} = \left(\hat{f} - a\hat{I}\right)^{+} \text{ if } a \in \mathbb{R}.$$

For the densely defined product of two symmetric operators, we have

$$\hat{f} \subseteq \hat{f}^{+},\ \hat{g} \subseteq \hat{g}^{+},\ \overline{D_{fg}} = \mathfrak{H} \Longrightarrow \hat{f}\hat{g} \subseteq \hat{f}^{+}\hat{g}^{+} \subseteq \left(\hat{g}\hat{f}\right)^{+},$$

the last inclusion becoming an equality if $\hat{g}$ is bounded and defined everywhere; in general, the product of two symmetric operators is not symmetric, but if $\hat{f}$ is bounded and defined everywhere, $D_f = \mathfrak{H}$, and if $\hat{f}$ and $\hat{g}$ commute, $\hat{f}\hat{g} \subseteq \hat{g}\hat{f}$ (see Sect. 2.3.4), then the product $\hat{f}\hat{g}$ is symmetric:

$$\hat{f}\hat{g} \subseteq \hat{g}\hat{f} \subseteq \hat{g}^{+}\hat{f}^{+} \subseteq \left(\hat{f}\hat{g}\right)^{+}.$$

2.7.3 Symmetricity and Extensions

We start with a simple assertion, which is very important in what follows.

Lemma 2.53. *If a symmetric operator $\hat{f}$ allows a symmetric extension $\hat{g}$, $\hat{f} \subseteq \hat{g}$, with $\hat{g} \subseteq \hat{g}^{+}$, then the chain of inclusions*

$$\hat{f} \subseteq \hat{g} \subseteq \hat{g}^{+} \subseteq \hat{f}^{+}$$

holds.

The proof follows directly from Lemma 2.40.

By Lemma 2.53, a densely defined restriction $\hat{f}_0$ of a symmetric operator $\hat{f}$ is also symmetric: $\hat{f}_0 \subseteq \hat{f} \subseteq \hat{f}^+ \subseteq \hat{f}_0^+$. If the adjoint $\hat{f}_0^+$ of $\hat{f}_0$ is easily evaluated, we can evaluate the adjoint $\hat{f}^+$ of $\hat{f}$ using Remark 2.41 in Sect. 2.6.2. A symmetric operator $\hat{f}$ not identical with its adjoint, $\hat{f} \subset \hat{f}^+$ (a strict inclusion), is called a *maximal symmetric operator* if it does not allow a symmetric extension:

$$\hat{f} \subseteq \hat{g} \subseteq \hat{g}^+ \subseteq \hat{f}^+ \Longrightarrow \hat{g} = \hat{f}.$$

Different chains of successive symmetric extensions $\hat{g}, \ldots, \hat{h}$ of a given symmetric operator $\hat{f}$ are generally possible, resulting in chains of inclusions

$$\hat{f} \subseteq \hat{g} \subseteq \cdots \subseteq \hat{h} \subseteq \hat{h}^+ \subseteq \cdots \subseteq \hat{g}^+ \subseteq \hat{f}^+.$$

In these chains, successive symmetric extensions are accompanied by successive restrictions of the respective adjoint operators, so that the extensions and their adjoints "go to meet each other." We note in advance that an alternative holds: for all the chains of symmetric extensions of a given symmetric $\hat{f}$, either the final extension and its adjoint coincide, $\hat{h} = \hat{h}^+$, i.e., the procedure of symmetrically extending ends with an s.a. operator, or any chain ends with a maximal symmetric operator, i.e., with a strict inclusion $\hat{h} \subset \hat{h}^+$. This is the subject of the theory of s.a. extensions of symmetric operators; see Chap. 3.

2.7.4 Symmetricity, Closability, and Closure

Lemma 2.54. *A symmetric operator $\hat{f}$ is closable, its closure $\overline{\hat{f}}$ is a symmetric operator, and the chain of inclusions*

$$\hat{f} \subseteq \overline{\hat{f}} = \left(\hat{f}^+\right)^+ \subseteq \left(\overline{\hat{f}}\right)^+ = \hat{f}^+$$

holds.

Proof. Any symmetric operator $\hat{f}$ is closable because it has a closed extension $\hat{f}^+$. Its closure $\overline{\hat{f}}$ is the minimum closed extension of $\hat{f}$, which yields $\hat{f} \subseteq \overline{\hat{f}} \subseteq \hat{f}^+$. By Lemma 2.40, it follows that $(\hat{f}^+)^+ \subseteq (\overline{\hat{f}})^+ \subseteq \hat{f}^+$, and it remains to refer to Lemmas 2.42 and 2.43 to obtain the required chain of inclusions. □

It follows from Lemma 2.54 that a maximal symmetric operator is closed because it is identical with its symmetric extension, which is its closure.

2.7.5 Symmetricity and Invertibility

Lemma 2.55. *For a symmetric operator $\hat{f}$,*

(i) its kernel belongs to the kernel of its adjoint, $\ker \hat{f} \subseteq \ker \hat{f}^{+}$*, and*
(ii) if $\ker \hat{f}^{+} = \{0\}$*, then $\hat{f}$ is invertible, its inverse $\hat{f}^{-1}$ is symmetric, and we have $\hat{f}^{-1} \subseteq (\hat{f}^{-1})^{+} = (\hat{f}^{+})^{-1}$.*

Proof. The first assertion is obvious. As to the second assertion, its proof reduces to references to Lemma 2.28 and Lemma 2.48. □

We note that if $\ker \hat{f}^{+} \neq \{0\}$, it may be that $\ker \hat{f} = \{0\}$ and $\hat{f}$ is invertible. But in this case, the inverse $\hat{f}^{-1}$ is not symmetric: $\overline{D_{f^{-1}}} = \overline{R_f} = (\ker \hat{f}^{+})^{\perp} \neq \mathfrak{H}$, and therefore, the adjoint $(\hat{f}^{-1})^{+}$, as well as $(\hat{f}^{+})^{-1}$, does not exist.

2.7.6 Spectrum, Deficient Subspaces, and Deficiency Indices

We first note that by Lemmas 2.54 and 2.35, the spectra of a symmetric operator and of its closure, which is also symmetric, are the same and are closed sets.

Lemma 2.56. *The eigenvalues of a symmetric operator $\hat{f}$ are real-valued, and the eigenvectors corresponding to different eigenvalues are orthogonal.*

Proof. A proof can be found in any textbook on QM. First, we have

$$\hat{f}\xi_\lambda = \lambda\xi_\lambda \Longrightarrow \left(\xi_\lambda, \hat{f}\xi_\lambda\right) = \lambda\,(\xi, \xi) = \lambda\|\xi_\lambda\|^2\,,$$

and because $(\xi, \hat{f}\xi)$ is real, it follows that λ is real, $\lambda = \overline{\lambda}$. Second, we have

$$\begin{aligned} &\hat{f}\xi_{\lambda_1} = \lambda_1\xi_{\lambda_1},\ \hat{f}\xi_{\lambda_2} = \lambda_2\xi_{\lambda_2},\ \xi_{\lambda_1}, \xi_{\lambda_2} \in D_f\,, \\ &\qquad \Longrightarrow 0 = \left(\xi_{\lambda_1}, \hat{f}\xi_{\lambda_2}\right) - \left(\hat{f}\xi_{\lambda_1}, \xi_{\lambda_2}\right) = (\lambda_2 - \lambda_1)\,(\xi_{\lambda_1}, \xi_{\lambda_2}), \end{aligned}$$

which yields $(\xi_{\lambda_1}, \xi_{\lambda_2}) = 0$ for $\lambda_1 \neq \lambda_2$. □

In some textbooks on QM for physicists, this statement is formulated for s.a. operators with the conclusion that the spectrum of such operators is real-valued and the corresponding eigenvectors form an orthonormal basis. We see that this statement also holds for symmetric operators that are not s.a. in the general case, but—more importantly—eigenvalues generally do not form the whole spectrum (it may be that there are no eigenvalues at all).

According to Sect. 2.5, a number λ is a point of the spectrum of an operator $\hat{f}$ if either:

(i) The operator $\hat{\mathcal{R}}(\lambda)$ does not exist, or, which is the same, λ is an eigenvalue of $\hat{f}$, or
(ii) The operator $\hat{\mathcal{R}}(\lambda)$ exists, but is unbounded, or
(iii) The operator $\hat{\mathcal{R}}(\lambda)$ exists and is bounded, but is not densely defined, $\overline{D_{\mathcal{R}(\lambda)}} = \overline{R_{f(\lambda)}} \neq \mathfrak{H}$ (if $\hat{f}$ is closed, we have $D_{\mathcal{R}(\lambda)} = \overline{D_{\mathcal{R}(\lambda)}}$ by Lemma 2.32).

We briefly discuss different possibilities for a number $z \in \mathbb{C}$ to be a point of the spectrum of a symmetric operator $\hat{f}$ or to be a regular point.

By Lemma 2.56, the operator $\hat{\mathcal{R}}(z)$ may not exist (case (i)) only for real z that are the eigenvalues of $\hat{f}$ (again, the set of eigenvalues may be empty). Cases (ii) and (iii) are possible for real z as well, and regular points may also belong to the real axis.

As for complex numbers z with nonzero imaginary part, the following assertions hold.[20]

Lemma 2.57. *Let $\hat{f}$ be a symmetric operator, and let z be a complex number with nonzero imaginary part, $z \in \mathbb{C}'$. Then the operator $\hat{f}(z)$ is invertible, its inverse $\hat{\mathcal{R}}(z)$ is bounded with $\|\hat{\mathcal{R}}(z)\| \leq |y|^{-1}$, and if $\hat{f}$ is a closed operator, the domain of $\hat{\mathcal{R}}(z)$, which is the range of $\hat{f}(z)$, is a closed subspace:*

$$D_{\mathcal{R}(z)} = R_{f(z)} = \overline{R_{f(z)}} = \overline{D_{\mathcal{R}(z)}}.$$

Proof. The first assertion follows directly from Lemma 2.56 (we already know this). For a symmetric operator $\hat{f}$ and a complex number $z = x + iy$, we have the equality

$$\left\|\hat{f}(z)\,\xi\right\|^2 = \left(\hat{f}(x)\,\xi - iy\xi, \hat{f}(x)\,\xi - iy\xi\right) = \left\|\hat{f}(x)\,\xi\right\|^2 + y^2\,\|\xi\|^2\,,\ \forall \xi \in D_f$$

(the cross terms cancel), and therefore the inequality $\|\hat{f}(z)\xi\| \geq |y|\,\|\xi\|$ holds. The second assertion of the lemma then follows from Lemma 2.27. The third assertion follows from Lemma 2.32 (we also noted this above). □

It follows from Lemma 2.57 that a complex number $z \in \mathbb{C}'$ can be either a regular point of a symmetric operator $\hat{f}$ or a point of its spectrum (case (iii)). To distinguish the possibilities, we refer to Lemma 2.46 and (2.26), according to which

$$\mathfrak{H} = \overline{R_{f(z)}} \oplus \ker \hat{f}^{+}(\bar{z}) = \overline{D_{\mathcal{R}(z)}} \oplus \ker \hat{f}^{+}(\bar{z}),$$

and therefore, the operator $\hat{\mathcal{R}}(z)$ is densely defined iff $\ker \hat{f}^{+}(\bar{z}) = \{0\}$, while $\hat{\mathcal{R}}(z)$ is not densely defined iff $\ker \hat{f}^{+}(\bar{z}) \neq \{0\}$.

[20] Some of the assertions are already known; we collect them for future reference.

We thus obtain that a complex number $z \in \mathbb{C}'$ is a regular point of a symmetric operator $\hat{f}$ iff $\bar{z}$ is not an eigenvalue of the adjoint $\hat{f}^+$, and z is a point of the spectrum of $\hat{f}$ iff $\bar{z}$ is an eigenvalue of $\hat{f}^+$; in other words, the complex part of the spectrum of a symmetric operator $\hat{f}$ coincides with the set of complex-conjugate eigenvalues of its adjoint $\hat{f}^+$. By the same arguments, this alternative holds for real $z = x$ if the operator $\hat{\mathcal{R}}(x)$ exists and is bounded; in particular, case (iii) is realized iff x is an eigenvalue of $\hat{f}^+$. We note that the above arguments actually show that for the general densely defined operator $\hat{f}$, a number λ is a point of its spectrum if the complex conjugate number $\overline{\lambda}$ is an eigenvalue of the adjoint operator $\hat{f}^+$, because in that case, $\overline{R_{f(\lambda)}} = (\ker \hat{f}^+(\overline{\lambda}))^\perp \neq \mathfrak{H}$, and even if $\hat{\mathcal{R}}(\lambda)$ exists and is bounded, it is not densely defined.

We now need some new notions.

For any operator $\hat{f}$, the orthogonal complement $\left(R_f\right)^\perp$ of its range is called the *deficient subspace* of the operator $\hat{f}$ (the "deficiency" is due to the impossibility of solving the equation $\hat{f}\xi = \eta$ if η belongs to the deficient subspace). The dimension $\dim \left(R_f\right)^\perp$ of the deficient subspace is called the *deficiency index* of the operator $\hat{f}$.

In the case of finite-dimensional spaces, the deficiency index of an operator (or its matrix) is the difference between the dimension of the space and the rank of the operator.

If an operator $\hat{f}$ is closable, the deficient subspaces and deficiency indices of $\hat{f}$ and of its closure $\overline{\hat{f}}$ are the same because of the obvious inclusions

$$R_f \subseteq R_{\bar{f}} \subseteq \overline{R_f} \Longrightarrow (R_f)^\perp = \left(\overline{R_f}\right)^\perp \supseteq (R_{\bar{f}})^\perp \supseteq \left(\overline{R_f}\right)^\perp,$$

where we use (2.2) and (2.3).

By Lemma 2.46, the deficient subspace of a densely defined operator $\hat{f}$ is the kernel of its adjoint, $\left(R_f\right)^\perp = \ker \hat{f}^+$, and therefore $\dim\ker \hat{f}^+$ is its deficiency index. We note that the equality $\hat{f}^+ = \left(\overline{\hat{f}}\right)^+$, see Lemma 2.42, shows that the deficient subspaces and deficiency indices of a densely defined operator $\hat{f}$ and of its closure $\overline{\hat{f}}$ are the same.

We now return to symmetric operators, which are densely defined by definition and at the same time are closable by Lemma 2.54. In our case of the operator $\hat{f}(z) = \hat{f} - z\hat{I}$ with a varying complex number z, it is reasonable to call the deficient subspace and the deficiency index of this operator the deficient subspace and the deficiency index of the operator $\hat{f}$ corresponding to the complex number z.

Let $m(z)$ denote this deficiency index,

$$m(z) = \dim \left(R_{f(z)}\right)^\perp = \dim\ker \hat{f}^+(\bar{z}).$$

If z is a regular point of $\hat{f}$, the respective deficient subspace is trivial, and $m(z) = 0$. If $z \in \mathbb{C}'$, the converse holds: $m(z) = 0$ implies that z is a regular point of $\hat{f}$. In the general case, it appears sufficient to distinguish the two cases: $z \in \mathbb{C}_-$, the lower complex half-plane, and $z \in \mathbb{C}_+$, the upper complex half-plane.

Theorem 2.58. *For a symmetric operator $\hat{f}$, the deficiency index $m(z)$ is a constant m_+ independent of z in the lower half-plane $\mathbb{C}_-$ and is a constant m_- independent of z in the upper half-plane $\mathbb{C}_+$,*

$$m(z) = \begin{cases} m_+, & z \in \mathbb{C}_-, \\ m_-, & z \in \mathbb{C}_+. \end{cases}$$

In general, m_+ and m_- are different, but if there is a real point x such that $\hat{\mathcal{R}}(x)$ exists and is bounded, then $m_\pm = m = \dim\ker \hat{f}^+(x)$.

We call attention to the anticorrespondence between the subscripts $+$ and $-$ of $m_\pm$ and the sign of the imaginary part y of $z = x + iy$; the correspondence is with $\bar{z} = x - iy$. The numbers $m_\pm$ are called the *deficiency indices of a symmetric operator* $\hat{f}$ corresponding to the respective lower half-plane $\mathbb{C}_-$ and upper half-plane $\mathbb{C}_+$.

This theorem has a topological nature: as z continuously changes in $\mathbb{C}_-$ or $\mathbb{C}_+$, the operator $\hat{\mathcal{R}}(z)$ remains bounded and changes continuously; the deficient subspace only "rotates" without any jumps of its dimension, which is an integer or infinity (two infinite-dimensional subspaces are considered to be of equal dimension), and if this operator remains bounded at some point of the real axis, then m_+ and m_- are equal.

Proof. The proof is a modification of the proof of Lemma 2.35. Let $z \in \mathbb{C}_-$. We first note that the bounded operator $\hat{\mathcal{R}}(z)$ can be extended from its domain $D_{\mathcal{R}(z)} = R_{f(z)}$ to the whole of $\mathfrak{H}$ with the same norm[21] (see Lemma 2.21). Let $\hat{r}_z$ be such an extension:[22]

$$\hat{\mathcal{R}}(z) \subseteq \hat{r}_z, \;\; D_{r_z} = \mathfrak{H}, \;\; \|\hat{r}_z\| = \left\|\hat{\mathcal{R}}(z)\right\| \le |y|^{-1}.$$

According to Lemma 2.26, we have $\hat{I}_{D_f} = \hat{\mathcal{R}}(z)\,\hat{f}(z) = \hat{r}_z \hat{f}(z)$.

We now examine the operator $\hat{f}(z + \delta z)$, where $|\delta z| < |y| \le \|\hat{\mathcal{R}}(z)\|^{-1} = \|\hat{r}_z\|^{-1}$, such that $z + \delta z \in \mathbb{C}_-$ and $|\delta z|\,\|\hat{r}_z\| < 1$. This operator allows the representation

$$\hat{f}(z + \delta z) = \hat{f}(z) - \delta z \hat{I}_{D_f} = (\hat{I} - \delta z \hat{r}_z)\hat{f}(z).$$

The operator $\hat{I} - \delta z\,\hat{r}_z$ is a sum of two bounded operators defined everywhere, which allows successively using (2.26), (2.28), and (2.25) to find

$$(\hat{f}(z + \delta z))^+ = \hat{f}^+(\overline{z + \delta z}) = \hat{f}^+(\bar{z})(\hat{I} - \overline{\delta z}\,\hat{r}_z^+),$$

[21] Without loss of generality, we can assume $\hat{f}$ to be closed; then the domain of $\hat{\mathcal{R}}(z)$ is closed.

[22] If $\hat{\mathcal{R}}(z)$ is densely defined, the point z is a regular point, and $\hat{\mathcal{R}}(z)$ is the resolvent of $\hat{f}$ at the point z.

where by Lemma 2.39 the operator $\hat{r}_z^+$, the adjoint of $\hat{r}_z$, is defined everywhere and bounded with $\left\|\hat{r}_z^+\right\| = \|\hat{r}_z\|$. Because $\left\|-\overline{\delta z}\,\hat{r}_z^+\right\| = |\delta z|\,\|\hat{r}_z\| < 1$, the operator $\hat{I} - \overline{\delta z}\,\hat{r}_z^+$ satisfies the conditions of Lemma 2.31. By this lemma, the operator $\hat{I} - \overline{\delta z}\,\hat{r}_z^+$ is invertible, and its inverse is also bounded and defined everywhere. It follows that the kernels of the operators $\hat{f}^+(\overline{z+\delta z})$ and $\hat{f}^+(\overline{z})$ are of the same dimension,[23] i.e., $m(z+\delta z) = m(z)$.

We thus obtain that in an open circle around any point $z \in \mathbb{C}_-$ of radius $\varepsilon < |y|$, the deficiency index of a symmetric operator $\hat{f}$ is constant. To prove that $m(z) = m_+ = \text{const}$ in the whole half-plane $\mathbb{C}_-$, it is sufficient to invoke the Heine–Borel theorem: we connect any two points of $\mathbb{C}_-$ with a straight line and cover it by a finite number of intersecting open circles where the deficiency index is constant.

A proof for the upper half-plane is quite similar. The same argument shows that if there exists a real point x such that the operator $\hat{\mathcal{R}}(x)$ exists and is bounded, then there exists an open circle around this point of radius $\varepsilon < \|\hat{\mathcal{R}}(x)\|^{-1}$ where the deficiency index of $\hat{f}$ is a constant $m = m(x)$, which implies that $m_\pm = m$. □

In particular, if a real x is a regular point of a symmetric operator $\hat{f}$, then its deficiency indices are equal to zero, $m_\pm = 0$. Conversely, if at least one of the deficiency indices of $\hat{f}$ differs from zero, there can be no regular points of $\hat{f}$ on the real axis, and the real axis, as a whole, belongs to the spectrum of the operator $\hat{f}$. We can confirm the last assertion in a different way. If $m_+ \neq 0$ or $m_- \neq 0$, the spectrum of $\hat{f}$ must contain the half-plane $\mathbb{C}_-$ or $\mathbb{C}_+$ respectively together with its boundary, the real axis, because the spectrum of $\hat{f}$ is a closed set.

Corollary 2.59. *If a densely defined operator $\hat{f}$ is bounded from below or from above, it is symmetric and its deficiency indices coincide; if both its deficiency indices are equal to zero, $m_\pm = 0$, then spec $\hat{f} \subseteq [a,\infty)$ for $\hat{f} \geq a\hat{I}$ and spec $\hat{f} \subseteq (-\infty, b]$ for $\hat{f} \leq b\hat{I}$.*

The first assertion is a paraphrase of Corollary 2.51. According to Theorem 2.58, it is then sufficient to indicate a point x of the real axis such that the operator $\hat{\mathcal{R}}(x)$ exists and is bounded. Let, for example, $\hat{f} \geq a\hat{I}$, $a = \overline{a}$, i.e., $(\xi, \hat{f}(a)\xi) \geq 0$, $\forall \xi \in D_f$. For $x < a$, we have

$$\left(\xi, \hat{f}(x)\,\xi\right) = \left(\xi, \hat{f}(a)\,\xi\right) + (a-x)\,(\xi,\xi) \geq (a-x)\,\|\xi\|^2\,,\ \ \forall \xi \in D_f\,.$$

On the other hand, $(\xi, \hat{f}(x)\xi) \leq \|\hat{f}(x)\xi\|\,\|\xi\|$ because of the Cauchy–Schwarz inequality, which yields

$$\left\|\hat{f}(x)\,\xi\right\| \geq (a-x)\,\|\xi\|\,,\ \ a-x > 0,\ \ \forall \xi \in D_f.$$

[23]If two operators $\hat{g}$ and $\hat{h}$ are related by $\hat{g} = \hat{h}\hat{s}$, where $\hat{s}$ is defined everywhere and invertible and $\hat{s}^{-1}$ is also defined everywhere, the kernels of these operators are related by $\ker \hat{g} = \hat{s}^{-1} \ker \hat{h}$ and $\ker \hat{h} = \hat{s} \ker \hat{g}$, which implies that the kernels are of the same dimension.

By virtue of Lemma 2.27, it follows that the operator $\hat{\mathcal{R}}(x)$ exists and is bounded for all $x < a$. If, in addition, $m_{\pm} = 0$, the points $x < a$ are the regular points of $\hat{f}$ together with the complex points $z \in \mathbb{C}'$, and the spectrum of $\hat{f}$ belongs to the real semiaxis on the right of a: spec $\hat{f} \subseteq [a, \infty)$.

The case $\hat{f} \leq b\hat{I}$, $b = \overline{b}$, is considered similarly.

We notice once again that the deficiency indices of a symmetric operator and of its closure are the same.

We outline different possibilities for the deficiency indices $m_{\pm}$ and for the spectrum of a symmetric operator $\hat{f}$. The following variants are possible:

(i) $m_{\pm} = 0$, i.e., the adjoint $\hat{f}^{+}$ has no complex eigenvalues and $\overline{R_{f(z)}} = \mathfrak{H}$, Im $z \neq 0$, which, in particular, holds in the case of $\hat{f} = \hat{f}^{+}$; both half-planes $\mathbb{C}_{-}$ and $\mathbb{C}_{+}$ belong to the resolvent set, while the spectrum of $\hat{f}$ is real-valued, spec $\hat{f} \subseteq \mathbb{R}$.

(ii) $m_{+} = 0$, $m_{-} \neq 0$, i.e., the adjoint $\hat{f}^{+}$ has complex eigenvalues that fill $\mathbb{C}_{+}$; $\mathbb{C}_{-}$ belongs to the resolvent set, while $\mathbb{C}_{+}$ belongs to the spectrum of $\hat{f}$ together with the real axis (since the spectrum is a closed set), regp $\hat{f} = \mathbb{C}_{-}$ and spec $\hat{f} = \mathbb{R} \cup \mathbb{C}_{+}$.

(iii) $m_{+} \neq 0$, $m_{-} = 0$, i.e., the adjoint $\hat{f}^{+}$ has complex eigenvalues that fill $\mathbb{C}_{-}$; $\mathbb{C}_{+}$ belongs to the resolvent set, while $\mathbb{C}_{-}$ belongs to the spectrum of $\hat{f}$ together with the real axis, regp $\hat{f} = \mathbb{C}_{+}$ and spec $\hat{f} = \mathbb{R} \cup \mathbb{C}_{-}$.

(iv) $m_{\pm} \neq 0$, i.e., the adjoint $\hat{f}^{+}$ has complex eigenvalues filling $\mathbb{C}_{-}$and $\mathbb{C}_{+}$; $\mathbb{C}'$ belongs to the spectrum of $\hat{f}$ together with the real axis, which means that the spectrum of $\hat{f}$ is the whole complex plane, spec $\hat{f} = \mathbb{C}$. It may be that any $z \in \mathbb{C}$ is an eigenvalue of $\hat{f}^{+}$, whereas $\hat{f}$ has no eigenvalues; an example is presented in Sect. 6.1.3.

(v) If there is a point x of the real axis such that the operator $\hat{\mathcal{R}}(x)$ exists and is bounded, then the deficiency indices are equal, $m_{\pm} = m$; if there exists a regular point on the real axis, then the deficiency indices are equal to zero, $m_{\pm} = 0$.

2.8 Self-adjoint Operators

2.8.1 *Definitions and Properties*

Definition 2.60. A densely defined operator $\hat{f}$ is called a *self-adjoint operator* (*s.a. operator*) if it coincides with its adjoint, $\hat{f} = \hat{f}^{+}$. In the language of graphs, this means that $\mathbb{G}_{f} = \mathbb{G}_{f^{+}} = \left(\mathcal{E}\mathbb{G}_{f}\right)^{\perp}$. In the language of maps, this means that $\hat{f}$ is symmetric, and $D_{f} = D_{f^{+}}$.

The following criterion for self-adjointness is evident.

Lemma 2.61. *A symmetric operator $\hat{f}$ is s.a. iff $\xi_* \in D_{f^+} \Longrightarrow \xi_* \in D_f$, i.e.,*

$$\left(\xi_*, \hat{f}\xi\right) = \left(\hat{f}^+\xi_*, \xi\right), \ \forall\xi \in D_f \Longrightarrow \xi_* \in D_f.$$

To make sure that an operator $\hat{f}$ is s.a., we can verify that (1) $\hat{f}$ is symmetric and that (2) the criterion of Lemma 2.61 holds.

It is not infrequent that a physicist easily verifies (1), but forgets about (2), which must never be forgotten. Physical QM observables must be represented by s.a. operators, and not simply symmetric ones. Only s.a. operators possess the remarkable properties of a real-valued spectrum and a complete orthogonal system of (in general "generalized") eigenvectors corresponding to this spectrum, which provides the possibility of a probabilistic physical interpretation of QM states, observables, and measurements.

Regarding the relationship between self-adjointness to all other previous notions, all properties of adjoint and symmetric operators listed in the previous sections are valid for s.a. operators, sometimes in evidently weaker or stronger forms. We only cite them with brief remarks and references.

Lemma 2.62. *All means of an s.a. operator $\hat{f}$ are real, $(\xi, \hat{f}\xi) = \overline{(\xi, \hat{f}\xi)}$, $\forall\xi \in D_f$, and determine the norm of the operator,*

$$\left\|\hat{f}\right\| = \sup_{\xi\in D_f,\, \|\xi\|=1} \left|\left(\xi, \hat{f}\xi\right)\right|.$$

These assertions are the respective paraphrases of the necessary condition of item (ii) of Lemma 2.50 and the last equality in (2.30) of Lemma 2.52.

The first property is well known to physicists. The last equality is evident for physicists: the norm of an s.a. operator $\hat{f}$ is determined by its eigenvalue of maximum modulus in view of the following (naïve) expansions with respect to the complete orthonormalized system $\{e_k\}_1^\infty$ of eigenvectors of $\hat{f}$:

$$\xi = \sum_k a_k e_k, \ \|\xi\| = \sum_k |a_k|^2; \ \hat{f}\xi = \sum_k \lambda_k a_k e_k, \ \left\|\hat{f}\xi\right\| = \sum_k \lambda_k^2 |a_k|^2.$$

2.8.2 Self-adjointness and Algebra

As for symmetric operators, the algebraic properties of s.a. operators follow from the relation between the adjoint operation and algebra presented in Sect. 2.6.5.

Lemma 2.63. *The following relations hold for s.a. operators:*

(i) $\hat{f} = \hat{f}^{+}, a \in R \Longrightarrow a\hat{f} = (a\hat{f})^{+}$, $D_{af} = D_f$.

(ii) $\hat{f} = \hat{f}^{+}$, $\hat{g} = \hat{g}^{+}$, $\overline{D_f \cap D_g} = \mathfrak{H} \Longrightarrow (\hat{f} + \hat{g})^{+} \supseteq \hat{f} + \hat{g}$. *In general, the sum* $\hat{f} + \hat{g}$ *of two s.a. operators is no more than symmetric if densely defined, but if one of the operators, let it be* $\hat{g}$, *is defined everywhere, and is therefore bounded,*[24] *then the sum is an s.a. operator,* $\hat{f} + \hat{g} = (\hat{f} + \hat{g})^{+}$ *with* $D_{f+g} = D_f$.

(iii) $\hat{f} = \hat{f}^{+}$, $\hat{g} = \hat{g}^{+}$, $\overline{D_{fg}} = \mathfrak{H} \Longrightarrow (\hat{f}\hat{g})^{+} \supseteq \hat{g}\hat{f}$. *In general, the product* $\hat{f}\hat{g}$ *of two s.a. operators is not even symmetric; the product* $\hat{f}\hat{g}$ *is symmetric,* $(\hat{f}\hat{g})^{+} \supseteq \hat{f}\hat{g}$, *if* $\hat{f}$ *is defined everywhere, and is therefore bounded, and if* $\hat{g}\hat{f} \supseteq \hat{f}\hat{g}$, *i.e.,* $\hat{f}$ *and* $\hat{g}$ *commute; the product* $\hat{f}\hat{g}$ *is s.a.,* $(\hat{f}\hat{g})^{+} = \hat{f}\hat{g}$, *if both* $\hat{f}$ *and* $\hat{g}$ *are defined everywhere, and are therefore bounded, and commute,* $[\hat{f}, \hat{g}] = 0$.

The property (ii) is of particular importance for physics. If the unbounded s.a. "free" Hamiltonian $\hat{H}_0$ is perturbed by a bounded s.a. potential $\hat{V}$ defined everywhere, then the total Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ is s.a. with $D_H = D_{H_0}$. But if $\hat{V}$ is unbounded, then the sum $\hat{H}_0 + \hat{V}$ in general is no more than symmetric if densely defined, and we encounter the problem of its s.a. extension.

In contrast to the general unbounded operators, s.a. operators allow one to define the notion of their commutativity, which can be done in terms of the one-parameter family $\{\hat{U}_f(\alpha) = \exp(\mathrm{i}\alpha\hat{f}),\ \alpha \in \mathbb{R}\}$ of mutually commuting unitary operators[25]

$$\left[\hat{U}_f(\alpha), \hat{U}_f(\beta)\right] = 0,\ \forall \alpha, \beta \in \mathbb{R},$$

associated with each s.a. operator $\hat{f}$. Self-adjoint operators $\hat{f}$ and $\hat{g}$ are called commuting, or commute, if the respective families $\{\hat{U}_f(\alpha)\}$ and $\{\hat{U}_g(\alpha)\}$ of the associated unitary operators mutually commute: $[\hat{U}_f(\alpha), \hat{U}_g(\beta)] = 0$, $\forall \alpha, \beta \in \mathbb{R}$.

The families of associated unitary operators make it possible to formulate some nontrivial commutation relations for s.a. operators. For example, the canonical commutation relation $[\hat{q}, \hat{p}] = i\hbar$ for the position operator $\hat{q}$ and the momentum operator $\hat{p}$ is properly formulated as the Weil relation [128]

$$\hat{U}_q(\alpha)\,\hat{U}_p(\beta) = \mathrm{e}^{-\mathrm{i}\alpha\beta}\,\hat{U}_p(\beta)\,\hat{U}_q(\alpha),\ \forall \alpha, \beta \in \mathbb{R},$$

for the corresponding associated unitary operators $\hat{U}_q(\alpha) = \exp(\mathrm{i}\alpha\kappa_0\hat{q})$ and $\hat{U}_q(\beta) = \exp(\mathrm{i}\beta\hat{p}/\kappa_0\hbar)$, where κ_0 is a fixed parameter of dimension of inverse length.

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[24] According to Theorem 2.44; see also Lemma 2.67.

[25] We recall that unitary operators are bounded and defined everywhere, and the notion of commutativity for such operators is unambiguous; see Sect. 2.3.3.

2.8.3 Self-adjointness, Closability, and Extensions

Lemma 2.64. *An s.a. operator is closed, $\hat{f} = \hat{f}^{+} = \overline{\hat{f}}$, and allows no symmetric extensions.*

The proof reduces to citing Lemmas 2.42 and 2.53.

2.8.4 Self-adjointness and Invertibility

Lemma 2.65. *For an invertible s.a. operator, its range is dense in $\mathfrak{H}$, and its inverse is also s.a.,*

$$\hat{f} = \hat{f}^{+},\ \ker \hat{f} = \{0\} \Longrightarrow \overline{R_f} = \mathfrak{H} \text{ and } \hat{f}^{-1} = \left(\hat{f}^{-1}\right)^{+}.$$

The proofs of the first and second assertions directly follow from Corollary 2.47 and Lemma 2.48 respectively.

2.8.5 Symmetricity, Self-adjointness, and Boundedness

Lemma 2.66. *A bounded symmetric operator defined everywhere is s.a.:*

$$\hat{f} \subseteq \hat{f}^{+},\ D_f = \mathfrak{H},\ \|f\| < \infty \Longrightarrow \hat{f} = \hat{f}^{+}.$$

Proof. Indeed, the conditions $\hat{f} \subseteq \hat{f}^{+}$ and $D_f = \mathfrak{H}$ imply $D_{f^+} = \mathfrak{H}$; then see Lemma 2.61. □

We note that in fact, the boundedness of $\hat{f}$ is not involved; moreover, the boundedness can be moved from the conditions of the lemma to its conclusions, and we obtain a stronger assertion.

Lemma 2.67. *A symmetric operator defined everywhere is s.a. and bounded, in particular, an s.a. operator defined everywhere is bounded.*

We must prove only boundedness, but this immediately follows from Lemma 2.64 and Theorem 2.44.

Corollary 2.68. *An operator defined everywhere and bounded from above or from below is s.a. and bounded.*

It is sufficient to note that by Corollary 2.51, such an operator is symmetric.

Lemma 2.69. *A symmetric operator whose range coincides with the whole of $\mathfrak{H}$ is s.a. and invertible, and its inverse is s.a. and bounded:*

$$\hat{f} \subseteq \hat{f}^{+},\ R_f = \mathfrak{H} \Longrightarrow \ker \hat{f} = \{0\},\ \ \hat{f} = \hat{f}^{+},\ \ \hat{f}^{-1} = \left(\hat{f}^{-1}\right)^{+},\ \left\| \hat{f}^{-1} \right\| < \infty .$$

Proof. By the corollary to Lemma 2.46, the conditions $R_f = \mathfrak{H}$ and $\hat{f} \subseteq \hat{f}^{+}$ imply that $\hat{f}^{+}$ is invertible together with $\hat{f}$. By Lemma 2.55, the inverse $\hat{f}^{-1}$ is symmetric and therefore, by the previous Lemma 2.67, is s.a. and bounded since defined everywhere, $D_{f^{-1}} = R_f = \mathfrak{H}$. Then by Lemma 2.65, $\hat{f}$ itself is s.a. as the inverse of $\hat{f}^{-1}$. □

Corollary 2.70. *A positive (negative) operator whose range coincides with the whole of $\mathfrak{H}$ is s.a., and its inverse is s.a. and bounded.*

It is sufficient to prove that a positive (negative) operator $\hat{f}$ with $R_f = \mathfrak{H}$ is densely defined, $\overline{D_f} = \mathfrak{H}$, and is therefore symmetric by Corollary 2.51. Let $\eta \in D_f^{\perp}$, i.e., $(\xi, \eta) = 0, \forall \xi \in D_f$. Because $R_f = \mathfrak{H}$, the vector η allows the representation $\eta = \hat{f}\xi_\eta$ with some $\xi_\eta \in D_f$. For this ξ_η, we have $\left(\xi_\eta, \eta\right) = (\xi_\eta, \hat{f}\xi_\eta) = 0$, which implies for positive (negative) $\hat{f}$ that $\xi_\eta = 0$ and $\eta = 0, \forall \eta \in D_f^{\perp}$. This means that $D_f^{\perp} = \{0\}$, or $\overline{D_f} = \mathfrak{H}$.

Remark 2.71. We see that for operators defined everywhere, symmetricity is equivalent to self-adjointness and implies boundedness. But this is true only for such operators, which is sometimes hidden in textbooks on QM for physicists. An unbounded physical observable cannot be defined everywhere, and a proper choice of domains for unbounded physical observables providing their self-adjointness under quantization is one of the main problems in quantizing physical systems. In general, the choice of a domain is not unique if possible, and different possible choices result in different QM.

A simple geometric corollary of the above assertions can be useful. The condition $\hat{f} \subseteq \hat{f}^{+}$ implies the possibility of a symmetric extension for $\hat{f}$, while the condition $D_f = \mathfrak{H}$ implies that a nontrivial extension is possible only at the expense of the range R_f. But the property to be a graph is then violated for a nontrivial extension: two images would have one preimage. And $\hat{f}$ cannot be a maximal symmetric operator, because $\hat{f}$ is then a strict restriction of $\hat{f}^{+}$ and its domain must be smaller than $\mathfrak{H}$. According to similar geometric arguments, if $\hat{f}$ is symmetric, $\hat{f} \subseteq \hat{f}^{+}$, and its range coincides with the whole of $\mathfrak{H}$, $R_f = \mathfrak{H}$, a nontrivial symmetric extension is possible only at the expense of the domain D_f, but the property to be a graph is then violated for the inverse operator $\hat{f}^{-1}$, which exists and is bounded.

2.8.6 Spectrum. Essentially Self-adjoint Operators

An s.a. operator can be considered a particular case of a symmetric operator with zero deficiency indices; see item (i) in the end of Sect. 2.7.6. The general assertions concerning the spectrum of such operators are presented in that section. We collect them in a separate lemma as applied to s.a. operators, taking Lemma 2.62 into account.

Lemma 2.72. *The deficiency indices of an s.a. operator $\hat{f}$ are equal to zero, $m_{\pm} = 0$.*

The spectrum of an s.a. operator is real-valued, and its eigenvectors corresponding to different eigenvalues are orthogonal.[26]

If $\hat{f}$ is bounded from below, $\hat{f} \geq a\hat{I}$, $a = \overline{a}$, $|a| < \infty$, or from above, $\hat{f} \leq b\hat{I}$, $b = \overline{b}$, $|b| < \infty$, its spectrum is respectively bounded from below, spec $\hat{f} \subseteq [a\,, \infty)$, *or from above,* spec $\hat{f} \subseteq (-\infty\,, b]$. *If both conditions hold, $a\hat{I} \leq \hat{f} \leq b\hat{I}$, then* spec $\hat{f} \subseteq [a\,, b]$ *and the operator $\hat{f}$ is bounded, $\|\hat{f}\| \leq \max(|a|\,, |b|)$.*

If $\hat{f}$ is bounded, $\|\hat{f}\| = c < \infty$, then it is bounded from below and from above, $-c\hat{I} \leq \hat{f} \leq c\hat{I}$, and spec $\hat{f} \subseteq [-c, c]$.

The real-valuedness of the spectrum of any s.a. operator is equivalent to that any complex number $z = x + \mathrm{i}y$, $y \neq 0$, is a regular point. An additional restriction on the spectrum of an s.a. operator is the following criterion for a real number x to be a regular point of the operator and not a point of its spectrum.

Lemma 2.73. *A real number $x \in \mathbb{R}$ is a regular point of an s.a. operator $\hat{f}$ iff the range of the operator $\hat{f}(x) = \hat{f} - x\hat{I}$ is the whole Hilbert space $\mathfrak{H}$, $R_{f(x)} = \mathfrak{H}$, which is equivalent to that the equation $\hat{f}(x)\xi = (\hat{f} - x\hat{I})\xi = \eta$ with any $\eta \in \mathfrak{H}$ has a (unique) solution $\xi \in D_f$. In fact, this is a reduced definition of a real regular point for an s.a. operator.*

Proof. Because $\hat{f}$ is closed, a proof will be achieved by reference to Lemma 2.45 if we prove that the operator $\hat{f}\ (x)$ is invertible. But this is indeed the case, because $\hat{f}(x)$ is s.a. as well as $\hat{f}$, $\hat{f}(x) = (\hat{f}(x))^{+}$, and its kernel satisfies $\ker \hat{f}(x) = (R_{f(x)})^{\perp} = \{0\}$ by Lemma 2.46. □

The spectrum of an s.a. operator is not empty.[27] For s.a. operators, the following specification of the spectrum is conventional [9, 116]. As before, the set of all eigenvalues is called the point spectrum. The point spectrum of an s.a. operator in a separable Hilbert space (we recall that we restrict ourselves to such spaces) is finite or countable, because the eigenvectors corresponding to different eigenvalues are orthogonal, while any set of nonzero orthogonal vectors in a separable Hilbert space is at most countable; see Sect. 2.1.2.

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[26] It may be that an s.a. operator has no eigenvectors, in which case its spectrum is continuous.

[27] In contrast to the general closed operator, whose spectrum can be empty [128]. We also note that the spectrum of any bounded operator is not empty.

The union of the closure of the complement of the point spectrum in the whole spectrum and the eigenvalues of infinite multiplicity is called the *continuous spectrum*.[28] A point λ is the point of the spectrum of an s.a. operator $\hat{f}$ iff there exists an infinite orthonormalized set $\{\xi_n\}_1^\infty$ of vectors such that $(\hat{f} - \lambda\hat{I})\xi_n \longrightarrow 0$ as $n \longrightarrow \infty$. For the point spectrum, this assertion is trivial. As for the continuous spectrum, this assertion can be interpreted as an indication that a point of a continuous spectrum that is not an eigenvalue of infinite multiplicity is an "almost eigenvalue" of an s.a. operator.

The set of isolated points of the spectrum (they are eigenvalues) except the eigenvalues of infinite multiplicity is called the *discrete spectrum*.[29]

So, a real number λ belongs to the spectrum of an s.a. operator $\hat{f}$, $\lambda \in \operatorname{spec} \hat{f}$, if either:

(a) The operator $\hat{\mathcal{R}}(\lambda)$ does not exist, in which case λ is an eigenvalue of $\hat{f}$ and belongs to the point spectrum, or
(b) The operator $\hat{\mathcal{R}}(\lambda)$ exists, but is unbounded, in which case λ belongs to the continuous spectrum.

In the latter case, the operator $\hat{\mathcal{R}}(\lambda)$ is densely defined, but is not defined everywhere. Indeed, it cannot be defined everywhere because otherwise it would be bounded as a closed operator by Theorem 2.44, and it is densely defined because

$$\overline{D_{\mathcal{R}(\lambda)}} = \overline{R_{f(\lambda)}} = \left(\ker\left(\hat{f}(\lambda)\right)^+\right)^\perp, \text{ but } \ker\left(\hat{f}(\lambda)\right)^+ = \ker \hat{f}(\lambda) = \{0\}.$$

The situation (iii) from Sect. 2.7.6 that $\hat{\mathcal{R}}(\lambda)$ is bounded but not densely defined is thus excluded for an s.a. operator.

A subtlety is that λ may belong to the point spectrum and to the continuous spectrum simultaneously: an example is an eigenvalue of infinite multiplicity[30] or that an eigenvalue of finite multiplicity can lie in the continuous spectrum. The possibility of a continuous spectrum is a distinctive feature of s.a. operators in infinite-dimensional Hilbert spaces.

It appears that zero deficiency indices are not only a necessary condition for the self-adjointness of a symmetric operator, but also are an almost sufficient condition.

Definition 2.74. A symmetric operator $\hat{f}$ is called *an essentially s.a. operator* if its closure $\overline{\hat{f}}$ is s.a.

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[28] This classification is sufficient for our purposes. A more advanced classification can be found in [128].

[29] It may be an exotic situation whereby the point spectrum is dense in the continuous spectrum and the eigenvectors corresponding to the point spectrum form a complete orthonormalized set.

[30] For the identity operator $\hat{I}$, the point and continuous spectra coincide, reducing to the single eigenvalue $\lambda = 1$ of infinite multiplicity.

Lemma 2.75. *A symmetric operator is essentially s.a. iff its deficiency indices are equal to zero. In particular, a closed symmetric operator with zero deficiency indices is s.a.*

Proof. By Lemma 2.54, the closure $\overline{\hat{f}}$ of a symmetric operator $\hat{f}$ is symmetric, $\overline{\hat{f}} \subseteq \left(\overline{\hat{f}}\right)^{+} = \hat{f}^{+}$, and the deficiency indices of $\hat{f}$ and $\overline{\hat{f}}$ coincide. Therefore, it is sufficient to prove that if a closed symmetric operator $\hat{f}$ has zero deficiency indices, i.e., $\ker \hat{f}^{+}(z) = \{0\}$, $\forall z \neq \overline{z}$, then $\hat{f}$ is s.a. To prove this, we first note that by Lemma 2.57, the range of the operator $\hat{f}(z)$, $z \neq \overline{z}$, is closed, $R_{f(z)} = \overline{R_{f(z)}}$. Then by Lemma 2.46, we find that $R_{f(z)} = \mathfrak{H}$ because $\ker \hat{f}^{+}(\overline{z}) = \{0\}$, which means that any vector $\eta \in \mathfrak{H}$ allows the representation $\eta = \hat{f}(z)\,\xi$, where $\xi \in D_f$. In particular, for any vector $\xi_* \in D_{f^+}$, there exists some vector $\xi \in D_f$ such that $\hat{f}^{+}(z)\,\xi_* = \hat{f}(z)\,\xi$. But $\hat{f} \subseteq \hat{f}^{+}$ implies that $\hat{f}(z)\,\xi = \hat{f}^{+}(z)\,\xi$, and we obtain that $\hat{f}^{+}(z)\,\xi_* = \hat{f}^{+}(z)\,\xi$, or $\hat{f}^{+}(z)\,(\xi_* - \xi) = 0$, whence it follows that $\xi_* = \xi \in D_f$, $\forall \xi_* \in D_{f^+}$. It remains to refer to Lemma 2.61 to conclude that $\hat{f} = \hat{f}^{+}$. □

We thus obtain that a symmetric operator $\hat{f}$ with zero deficiency indices is either s.a., if $\hat{f}$ is closed, or allows an s.a. extension, if $\hat{f}$ is nonclosed. This s.a. extension is its closure $\overline{\hat{f}}$ coinciding with its adjoint $\hat{f}^{+}$ and is therefore unique because $\overline{\hat{f}}$ is a minimum closed symmetric extension of $\hat{f}$, whereas by Lemma 2.53, the operator $\hat{f}^{+}$ is a maximum possible symmetric extension. In other words, if the deficiency indices of a symmetric operator are equal to zero, then the operator is either s.a., if closed, or if nonclosed, allows a unique s.a. extension that is its adjoint.

As for symmetric operators with nonzero deficiency indices, their s.a. extensions are nonunique, if they exist at all, which is determined by the values of the deficiency indices. By analogy with an essentially s.a. operator, we call a symmetric operator $\hat{f}$ with nonzero deficiency indices an *essentially maximal symmetric operator* if its closure $\overline{\hat{f}}$ is a maximal symmetric operator. An essentially maximal symmetric operator has no s.a. extensions. This is the subject of Chap. 3.

We now consider some specific classes of s.a. operators that are of particular importance.

2.8.7 Orthoprojectors

An important class of bounded s.a. operators is a class of *orthoprojectors*. The notion of orthoprojector is a basic notion in the spectral analysis of s.a. operators; see Chap. 5 below.

Definition 2.76. Let $D \subseteq \mathfrak{H}$ be a closed subspace, $D = \overline{D}$. To each vector $\xi \in \mathfrak{H}$, we assign its projection on a closed subspace D; see Theorem 2.2.

This correspondence defines the operator that is called the *(ortho)projection operator* or *(ortho)projector* (on D), and is denoted by $\hat{P}$, or $\hat{P}_D$ if we stress that $\hat{P}$ is the orthoprojector just on D,

$$\hat{P} = \hat{P}_D = \begin{cases} D_P = \mathfrak{H}, \\ \hat{P}\xi = \xi_\parallel,\ \forall\xi \in \mathfrak{H}. \end{cases}$$

In particular, we have $\hat{P}_{\{0\}} = 0$, while $\hat{P}_{\mathfrak{H}} = \hat{I}$.

We cite the properties of orthoprojectors that directly follow from the definition.

1. Any orthoprojector $\hat{P}$ is a linear operator defined everywhere, $D_P = \mathfrak{H}$.
2. The range of the orthoprojector $\hat{P}_D$ is the subspace D, $R_{P_D} = D$.
3. $\ker \hat{P}_D = D^\perp$.
4. Any orthoprojector $\hat{P}$ is bounded, and its norm is equal to unity, $\|\hat{P}\| = 1$. Indeed, $\|\xi\|^2 = \left\|\xi_\parallel\right\|^2 + \|\xi_\perp\|^2$, $\forall\xi \in \mathfrak{H}$, which implies $\|\hat{P}\xi\|^2 = \left\|\xi_\parallel\right\|^2 \le \|\xi\|^2$, and equality is achieved for $\xi \in D = R_P$.
5. Any orthoprojector $\hat{P}$ is a nonnegative operator not exceeding the identity operator, $0 \le \hat{P} \le \hat{I}$. Indeed, $(\xi, \hat{P}\xi) = (\xi_\parallel + \xi_\perp, \xi_\parallel) = (\xi_\parallel, \xi_\parallel) \ge 0$, while
$$(\xi, (\hat{P} - \hat{I})\xi) = (\xi_\perp, -\xi_\perp) = -(\xi_\perp, \xi_\perp) \le 0.$$
6. If an operator $\hat{P}$ is the orthoprojector on a subspace D, $\hat{P} = \hat{P}_D$, then the operator $\hat{I} - \hat{P}$ is also an orthoprojector, namely, the orthoprojector on the subspace $D^\perp$, $\hat{I} - \hat{P}_D = \hat{P}_{D^\perp}$. Indeed, according to Corollary 2.3, we have $\hat{P}_{D^\perp}\xi = \xi_\perp = \xi - \xi_\parallel = (\hat{I} - \hat{P}_D)\xi$.
7. $\hat{P}^2 = \hat{P}$ for any orthoprojector $\hat{P}$, which means that its range R_P is the eigenspace of $\hat{P}$ with the eigenvalue $+1$: $\hat{P}\xi = \xi$, $\forall\xi \in R_P$. Indeed, $\hat{P}^2\xi = \hat{P}\xi_\parallel = \xi_\parallel$, $\forall\xi \in \mathfrak{H}$.
8. Any orthoprojector $\hat{P}$ is an s.a. operator, $\hat{P}^+ = \hat{P}$. It is sufficient to refer to Corollary 2.68.

   Properties 7 and 8 are the characteristic properties of orthoprojectors.

Theorem 2.77. *A linear operator $\hat{P}$ with the properties $\hat{P} = \hat{P}^+$ and $\hat{P}^2 = \hat{P}$ is the orthoprojector on the closed subspace $D = R_P$.*

Proof. We first prove that the operator $\hat{P}$ is bounded and defined everywhere. Using both properties of $\hat{P}$, we obtain

$$\left\|\hat{P}\xi\right\|^2 = (\hat{P}\xi, \hat{P}\xi) = (\hat{P}\hat{P}\xi, \xi) = (\hat{P}\xi, \xi) \le \left\|\hat{P}\xi\right\| \|\xi\|,\ \forall\xi \in D_P,$$

which implies that $\|\hat{P}\xi\| \le \|\xi\|$, $\forall\xi \in D_P$, i.e., $\hat{P}$ is bounded. But as an s.a. operator, $\hat{P}$ is densely defined, $\overline{D_P} = \mathfrak{H}$, and is closed, $\hat{P} = \overline{\hat{P}}$, together with the operator $\hat{I} - \hat{P}$. It then follows from Lemma 2.23 that $\hat{P}$ is defined everywhere, $D_P = \overline{D_P} = \mathfrak{H}$.

Let D denote the range R_P of $\hat{P}$, $D = R_P$, and let $D^{\perp}$ denote its orthogonal complement. We now prove that D is a closed subspace. The property $\hat{P}^2 = \hat{P}$ means that D is an eigenspace of $\hat{P}$ with the eigenvalue $+1$: $\hat{P}\xi = \xi$ if $\xi \in D$, or $D = \ker(\hat{I} - \hat{P})$ and is therefore closed as the kernel of a closed operator.

It follows that by Theorem 2.2, any vector $\xi \in \mathfrak{H}$ allows a uniquely defined decomposition $\xi = \xi_{\|} + \xi_{\perp}$, where $\xi_{\|} \in D$ is the projection of ξ on D, $\xi_{\|} = \hat{P}_D\xi$, and $\xi_{\perp} \in D^{\perp}$. Because $\hat{P}\xi_{\|} = \xi_{\|}$, we have $\hat{P}\xi = \xi_{\|} + \hat{P}\xi_{\perp}$, and it remains to prove that $\hat{P}\xi_{\perp} = 0$ to obtain that $\hat{P}\xi = \xi_{\|} = \hat{P}_D\xi$, $\forall\xi \in \mathfrak{H}$, which just means that $\hat{P} = \hat{P}_D$. But

$$\left\|\hat{P}\xi_{\perp}\right\|^2 = (\hat{P}\xi_{\perp}, \hat{P}\xi_{\perp}) = (\xi_{\perp}, \hat{P}\hat{P}\xi_{\perp}) = (\xi_{\perp}, \hat{P}\xi_{\perp}) = 0,$$

because $\hat{P}\xi_{\perp} \in D$, which completes the proof. □

The following is a collection of assertions concerning the product, addition, and subtraction of orthoprojectors.

Lemma 2.78. *The product of two orthoprojectors $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ is an orthoprojector, $\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}$, iff $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ commute, $\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$, and if this condition holds, then $\hat{P} = \hat{P}_D$, where $D = D_1 \cap D_2$.*

Proof. Necessity. Let the product of two orthoprojectors $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ be an orthoprojector, $\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}$. The equality $\hat{P} = \hat{P}^2 = \hat{P}^+$ then yields

$$\hat{P}_{D_1}\hat{P}_{D_2} = \left(\hat{P}_{D_1}\hat{P}_{D_2}\right)^+ = \hat{P}^+_{D_2}\hat{P}^+_{D_1} = \hat{P}_{D_2}\hat{P}_{D_1},$$

i.e., $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ commute.

Sufficiency. Let two orthoprojectors $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ commute. The operator $\hat{P} = \hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$ evidently satisfies the conditions of Theorem 2.77:

$$\hat{P}^+ = \left(\hat{P}_{D_1}\hat{P}_{D_2}\right) = \hat{P}^+_{D_2}\hat{P}^+_{D_1} = \hat{P}_{D_2}\hat{P}_{D_1} = \hat{P}$$

and

$$\hat{P}^2 = \hat{P}_{D_1}\hat{P}_{D_2}\hat{P}_{D_2}\hat{P}_{D_1} = \hat{P}_{D_1}\hat{P}_{D_2}\hat{P}_{D_1} = \hat{P}_{D_1}\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_1}\hat{P}_{D_2} = \hat{P},$$

whence it follows that $\hat{P}$ is an orthoprojector.

We know that $\hat{P} = \hat{P}_D$, where $D = R_P = \{\hat{P}\xi, \forall\xi \in \mathfrak{H}\} = \{\xi : \hat{P}\xi = \xi\}$. According to the first representation $\hat{P} = \hat{P}_{D_1}\hat{P}_{D_2}$, we have $\hat{P}\xi = \hat{P}_{D_1}\hat{P}_{D_2}\xi \in D_1$, while according to the second representation $\hat{P} = \hat{P}_{D_2}\hat{P}_{D_1}$, we have $\hat{P}\xi = \hat{P}_{D_2}\hat{P}_{D_1}\xi \in D_2$, which implies that $D \subseteq D_1 \cap D_2$. Conversely, let $D \in D_1 \cap D_2$. Then we have $\xi = \hat{P}_{D_1}\xi = \hat{P}_{D_2}\xi = \hat{P}_{D_1}\hat{P}_{D_2}\xi = \hat{P}\xi$, which implies that $D_1 \cap D_2 \subseteq D$, and therefore, $D = D_1 \cap D_2$.

Corollary 2.79. *Two closed subspaces D_1 and D_2 are orthogonal, $D_1 \perp D_2$, iff $\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1} = \hat{0}$.* □

A geometric sense of the equality $\hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$ is that the closed subspaces $D_1 \ominus (D_1 \cap D_2)$ and $D_2 \ominus (D_1 \cap D_2)$ are orthogonal, because if equality holds, the operators $\hat{P}_{D_1}(\hat{I} - \hat{P}_{D_2})$ and $\hat{P}_{D_2}(\hat{I} - \hat{P}_{D_1})$ are orthoprojectors on the respective subspaces $D_1 \cap D_2^{\perp} = D_1 \ominus (D_1 \cap D_2)$ and $D_2 \cap D_1^{\perp} = D_2 \ominus (D_1 \cap D_2)$ and

$$(\hat{P}_{D_1}(\hat{I} - \hat{P}_{D_2}))(\hat{P}_{D_2}(\hat{I} - \hat{P}_{D_1})) = \hat{0}.$$

Lemma 2.80. *The sum of orthoprojectors $\hat{P}_j = \hat{P}_{D_j}$, $j = 1, \ldots, n < \infty$, is an orthoprojector, $\sum_{j=1}^{n} \hat{P}_j = \hat{P}$, iff the subspaces D_j are mutually orthogonal, i.e., iff $\hat{P}_j \hat{P}_k = 0$, $j \neq k$, and in this case, $\hat{P} = \hat{P}_D$, where $D = \sum_{j=1}^{n\,\oplus} D_j$.*

Proof. Necessity. Let the operator $\hat{P} = \sum_{j=1}^{n} \hat{P}_j$ be an orthoprojector. Then the inequalities

$$\begin{aligned}\|\xi\|^2 \geq (\xi, \hat{P}\xi) = \left(\xi, \sum_{j=1}^{n} \hat{P}_j \xi\right) &\geq (\xi, \hat{P}_j\xi) + (\xi, \hat{P}_k\xi) \\ &= \left\|\hat{P}_j\xi\right\|^2 + \left\|\hat{P}_k\xi\right\|^2, \ \forall\xi \in \mathfrak{H},\end{aligned}$$

hold whatever the different indices j and k may be. Taking $\xi = \hat{P}_k\eta$, we obtain that

$$\left\|\hat{P}_j\hat{P}_k\eta\right\|^2 + \left\|\hat{P}_k\eta\right\|^2 \leq \left\|\hat{P}_k\eta\right\|^2$$

and therefore $\|\hat{P}_j\hat{P}_k\eta\|^2 = 0$, $\forall\eta \in \mathfrak{H}$, which proves the equality $\hat{P}_j\hat{P}_k = 0$, or the orthogonality of the subspaces D_j and D_k, for $j \neq k$.

Sufficiency. If $\hat{P}_j\hat{P}_k = 0$, i.e., the subspaces D_j and D_k are mutually orthogonal, then evidently s.a. operator $\hat{P} = \sum_{j=1}^{n} \hat{P}_j$ satisfies the equality $\hat{P}^2 = \hat{P}$, and it remains to refer to Theorem 2.77. The last assertion of the lemma is also evident. □

Lemma 2.81. *The difference of two orthoprojectors $\hat{P}_{D_1}$ and $\hat{P}_{D_2}$ is an orthoprojector, $\hat{P}_{D_1} - \hat{P}_{D_2} = \hat{P}$, iff $D_2 \subseteq D_1$, which is equivalent to each of the relations $\hat{P}_{D_2} = \hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$, $\|\hat{P}_{D_2}\xi\| \leq \|\hat{P}_{D_1}\xi\|$ for $\forall\xi \in \mathfrak{H}$, and $\hat{P}_{D_2} \leq \hat{P}_{D_1}$, and in this case, $\hat{P} = \hat{P}_D$, where $D = D_1 \ominus D_2$.*

Proof. Necessity. Let $\hat{P}_{D_1} - \hat{P}_{D_2} = \hat{P}_D$, an orthoprojector on some D. Then the sum $\hat{P}_D + \hat{P}_{D_2} = \hat{P}_{D_1}$ is also an orthoprojector, and therefore by Lemma 2.80, $D_1 = D \oplus D_2$, which implies that $D_2 \subseteq D_1$ and $D = D_1 \ominus D_2$.

Sufficiency. Let $D_2 \subseteq D_1$, and let $D = D_1 \ominus D_2$. Then $D_1 = D \oplus D_2$, and therefore by Lemma 2.80, $\hat{P}_{D_1} = \hat{P}_D + \hat{P}_{D_2}$, or $\hat{P}_{D_1} - \hat{P}_{D_2} = \hat{P}_D$, which completes the proof.

It remains to prove the equivalence relations:

1. $D_2 \subseteq D_1 \Leftrightarrow \hat{P}_{D_2} = \hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1} = \hat{P}_{D_2}$.
   The relation $D_2 \subseteq D_1$ is evidently equivalent to the relation $\hat{P}_{D_2} = \hat{P}_{D_1}\hat{P}_{D_2}$, Lemma 2.78 allows extending the latter relation to $\hat{P}_{D_2} = \hat{P}_{D_1}\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$.
2. $D_2 \subseteq D_1 \Leftrightarrow \|\hat{P}_{D_2}\xi\| \leq \|\hat{P}_{D_1}\xi\|$, $\forall\xi \in \mathfrak{H}$.
   Let $D_2 \subseteq D_1$. Then $\hat{P}_{D_2} = \hat{P}_{D_2}\hat{P}_{D_1}$, which implies that
   $$\left\|\hat{P}_{D_2}\xi\right\| = \left\|\hat{P}_{D_2}\hat{P}_{D_1}\xi\right\| \leq \left\|\hat{P}_{D_2}\right\|\left\|\hat{P}_{D_1}\xi\right\| = \left\|\hat{P}_{D_1}\xi\right\|,\ \forall\xi \in \mathfrak{H}.$$
   Conversely, let $\|\hat{P}_{D_2}\xi\| \leq \|\hat{P}_{D_1}\xi\|$, $\forall\xi \in \mathfrak{H}$. Then the condition $\hat{P}_{D_1}\xi = 0$, or $\xi \in \ker\hat{P}_{D_1} = D_1^\perp$, implies that $\hat{P}_{D_2}\xi = 0$, or $\xi \in \ker\hat{P}_{D_2} = D_2^\perp$, which means that $D_1^\perp \subseteq D_2^\perp$, whence it follows that $D_2^\perp = (D_2^\perp)^\perp \subseteq (D_1^\perp)^\perp = D_1$.
3. $D_2 \subseteq D_1 \Leftrightarrow \hat{P}_{D_2} \leq \hat{P}_{D_1}$.
   In view of relation 2 above, it is sufficient to prove the equivalence of the inequalities
   $$\left\|\hat{P}_{D_2}\xi\right\| \leq \left\|\hat{P}_{D_1}\xi\right\|,\ \text{or}\ \left\|\hat{P}_{D_2}\xi\right\|^2 \leq \left\|\hat{P}_{D_1}\xi\right\|^2,\ \forall\xi \in \mathfrak{H},$$
   and $\hat{P}_{D_2} \leq \hat{P}_{D_1}$, or by definition, see the end of Sect. 2.3.1, $(\xi, \hat{P}_{D_2}\xi) \leq (\xi, \hat{P}_{D_1}\xi)$, $\forall\xi \in \mathfrak{H}$. But this equivalence directly follows from the equality $\|\hat{P}\xi\|^2 = (\hat{P}\xi, \hat{P}\xi) = (\xi, \hat{P}\xi)$, $\forall\xi \in \mathfrak{H}$, for any orthoprojector $\hat{P}$ in view of its basic properties $\hat{P}^+ = \hat{P}$ and $\hat{P}^2 = \hat{P}$. □

We complete this subsection with some simple assertions about sequences of orthoprojectors.

Lemma 2.82. *An infinite monotonic sequence $\{\hat{P}_k\}_1^\infty$ of orthoprojectors strongly converges to some orthoprojector $\hat{P}$.*

Proof. Let an operator sequence $\{\hat{P}_k\}_1^\infty$ be nondecreasing, $\hat{P}_k \leq \hat{P}_{k+1}$, i.e., $(\xi, \hat{P}_k\xi) \leq (\xi, \hat{P}_{k+1}\xi)$, $\forall\xi \in \mathfrak{H}$. Then the number sequence $\{(\xi, \hat{P}_k\xi)\}_1^\infty$ with any ξ is convergent as a nondecreasing bounded sequence, $0 \leq (\xi, \hat{P}_k\xi) \leq \|\xi\|^2$, and is therefore a Cauchy sequence, $(\xi, \hat{P}_n\xi) - (\xi, \hat{P}_m\xi) = (\xi, (\hat{P}_n - \hat{P}_m)\xi) \to 0$, $m, n \to \infty$. By Lemma 2.81, the difference $\hat{P}_n - \hat{P}_m$ is an orthoprojector up to a sign, which implies that $\|(\hat{P}_n - \hat{P}_m)\xi\|^2 = |(\xi, (\hat{P}_n - \hat{P}_m)\xi)|$. It follows that the vector sequence $\{\hat{P}_k\xi\}_1^\infty$ with any ξ is a Cauchy sequence and is therefore convergent, $\lim_{n\to\infty}\hat{P}_k\xi \to \hat{P}\xi$, where, as is easily seen, the operator $\hat{P}$ is linear, defined everywhere, and bounded. This means that the operator sequence $\{\hat{P}_k\}_1^\infty$ is strongly convergent to the operator $\hat{P}$. Taking then the limit $k \to \infty$ in the equalities

$$(\eta, \hat{P}_k\xi) = (\hat{P}_k\eta, \xi) = (\hat{P}_k\eta, \hat{P}_k\xi),\ \forall\xi, \eta \in \mathfrak{H},$$

we obtain that

$$(\eta, \hat{P}\xi) = (\hat{P}\eta, \xi) = (\hat{P}\eta, \hat{P}\xi), \ \forall \xi, \eta \in \mathfrak{H},$$

which means that $\hat{P} = \hat{P}^+ = \hat{P}^2$*, and therefore* $\hat{P}$ *is an orthoprojector by Theorem 2.77.* □

A proof for a nonincreasing sequence $\{\hat{P}_k\}_1^\infty$ of orthoprojectors, $\hat{P}_{k+1} \leq \hat{P}_k$, is completely similar

Lemma 2.83. *If the sequence* $\{\hat{P}_k\}_1^\infty$ *of orthoprojectors weakly converges to some orthoprojector* $\hat{P}$*, then it converges to* $\hat{P}$ *strongly.*

Proof. By the condition of the theorem, we have

$$(\eta, \hat{P}_k\xi) \to (\eta, \hat{P}\xi), \ k \to \infty, \ \forall \xi, \eta \in \mathfrak{H},$$

which in particular implies that

$$\left\| \hat{P}_k\xi \right\|^2 \to \left\| \hat{P}\xi \right\|^2, \ k \to \infty, \ \forall \xi \in \mathfrak{H}.$$

The proof follows directly from the equality

$$\left\| (\hat{P}_k - \hat{P})\xi \right\|^2 = \left\| \hat{P}_k\xi \right\|^2 - (\hat{P}_k\xi, \hat{P}\xi) - (\hat{P}\xi, \hat{P}_k\xi) + \left\| \hat{P}\xi \right\|^2.$$

□

2.8.8 Self-adjoint Operators of Oscillator Type

We call the operators of the form $\hat{N} = \hat{f}^+\hat{f}$ and $\hat{M} = \hat{f}\hat{f}^+$ *operators of oscillator type*. The name is due to the well-known oscillator Hamiltonian.

Many physicists and textbooks on QM for physicists consider these operators evidently s.a. Their arguments are based on the following commonly used formal rules for the Hermitian adjoint operation: $(\hat{f}^+)^+ = \hat{f}$ and $(\hat{f}^+\hat{f})^+ = \hat{f}^+(\hat{f}^+)^+ = \hat{f}^+\hat{f}$. However, we know that in general, these formal rules fail for unbounded operators: by Lemma 2.43, the operator $(\hat{f}^+)^+$ exists only for a closable operator $\hat{f}$, and $(\hat{f}^+)^+ = \overline{\hat{f}}$, which is not equal to $\hat{f}$ unless $\hat{f}$ is closed, while by (2.27), we generally have $(\hat{f}\hat{g})^+ \supseteq \hat{g}^+\hat{f}^+$. Fortunately, physicists are almost right, but a correct formulation and especially a proof need some nontrivial observations.

The following theorem is due to von Neumann [154]. In the proof of the theorem, we follow [9].

Theorem 2.84. *If an operator* $\hat{f}$ *is densely defined,* $\overline{D_f} = \mathfrak{H}$*, and closed,* $\hat{f} = \overline{\hat{f}}$*, then the operators* $\hat{N} = \hat{f}^+\hat{f}$ *and* $\hat{M} = \hat{f}\hat{f}^+$ *are s.a. and nonnegative,* $\hat{N} =$

$\hat{N}^{+} \geq 0$ *and* $\hat{M} = \hat{M}^{+} \geq 0$. *In addition,* $\ker \hat{N} = \ker \hat{f}$ *and* $\ker \hat{M} = \ker \hat{f}^{+}$*; consequently, if* $\ker \hat{f} \neq \{0\}$*, the operator* $\hat{N}$ *has a zero eigenvalue, whereas if* $\ker \hat{f} = \{0\}$*,* $\hat{N}$ *is positive, the same holds for the operator* $\hat{M}$ *with the substitution of* $\hat{f}^{+}$ *for* $\hat{f}$*.*

Proof. It is sufficient to prove the theorem for $\hat{N} = \hat{f}^{+}\hat{f}$, because for a closed $\hat{f}$, we have $\hat{f} = (\hat{f}^{+})^{+}$, and $\hat{M} = \hat{f}\hat{f}^{+}$ can be represented as $\hat{M} = (\hat{f}^{+})^{+}\hat{f}^{+}$, where $\hat{f}^{+}$ is closed. By Lemma 2.63, the operators $\hat{N}$ and $\hat{K} = \hat{N} + \hat{I}$ are s.a. or non-s.a. simultaneously. It is therefore sufficient to prove that $\hat{K} = \hat{K}^{+}$. By the corollary of Lemma 2.69, to do this, it is sufficient to prove that $\hat{K}$ is positive, $\hat{K} > 0$, and $R_K = \mathfrak{H}$. The positivity of $\hat{K}$ is evident. The operator $\hat{N} = \hat{f}^{+}\hat{f}$ is nonnegative for any $\hat{f}$, not necessarily closed:

$$\left(\xi, \hat{f}^{+}\hat{f}\xi\right) = \left(\hat{f}\xi, \hat{f}\xi\right) \geq 0\,, \ \forall \xi \in D_N \subseteq D_f,$$

whence it follows that $\hat{K} = \hat{N} + \hat{I} \geq \hat{I} > 0$.

We now prove that $R_K = \mathfrak{H}$. The central point of the proof is a geometric observation: $\hat{f} = \overline{\hat{f}}$ means that $\mathbb{G}_f = \overline{\mathbb{G}_f}$, which by (2.12) implies that $\overline{\mathcal{E}\mathbb{G}_f} = \mathcal{E}\mathbb{G}_f$, where the unitary operator $\mathcal{E}$ is given by (2.14), and therefore by (2.4) and (2.23), the decomposition

$$\mathbb{H} = \mathcal{E}\mathbb{G}_f \oplus \left(\mathcal{E}\mathbb{G}_f\right)^{\perp} = \mathcal{E}\mathbb{G}_f \oplus \mathbb{G}_{f^+}$$

holds. This decomposition means that for any pair of vectors $\eta, \zeta \in \mathfrak{H}$, the representation[31]

$$(\eta / -\zeta) = \left(\hat{f}\xi / -\xi\right) + \left(\xi_* / \hat{f}^{+}\xi_*\right) = \left(\hat{f}\xi + \xi_* / \hat{f}^{+}\xi_* - \xi\right)$$

holds with some $\xi \in D_f$ and $\xi_* \in D_{f^+}$, which are uniquely defined by η and ζ. If $\eta = 0$, we have $\xi_* = -\hat{f}\xi$ and obtain the representation

$$\zeta = \hat{f}^{+}\hat{f}\xi + \xi, \text{ or } \zeta = \left(\hat{N} + \hat{I}\right)\xi = \hat{K}\xi, \ \xi \in D_N = D_K \subseteq D_f,$$

for any $\zeta \in \mathfrak{H}$, which means that $R_K = \mathfrak{H}$. We have thus proved that $\hat{K}$ is s.a., and therefore, $\hat{N}$ is also s.a.

The remaining part of the theorem does not require that $\hat{f}$ be closed. It is evident that $\ker \hat{f} \subseteq \ker \hat{f}^{+}\hat{f}$: $\hat{f}\xi = 0$ automatically implies that $\hat{f}^{+}\hat{f}\xi = 0$. Conversely, $\hat{f}^{+}\hat{f}\xi = 0$ implies that $(\xi, \hat{f}^{+}\hat{f}\xi) = (\hat{f}\xi, \hat{f}\xi) = 0$, whence it follows

[31] The convenience of the minus sign in front of the vector ζ becomes clear below.

that $\hat{f}\xi = 0$, or $\ker \hat{f}^{+}\hat{f} \subseteq \ker \hat{f}$. Therefore, $\ker \hat{f}^{+}\hat{f} = \ker \hat{f}$. The equality $\ker \hat{f}^{+}\hat{f} = \ker \hat{f}^{+}$ is proved similarly. □

For a symmetric operator with nonzero deficiency indices, it may happen that the operator allows an extension of oscillator type with a closed cofactor, and therefore at least one s.a. extension of the operator exists. We note in advance that this implies that the operator has equal deficiency indices and allows different s.a. extensions if the deficiency indices differ from zero; see Chap. 3.

Chapter 3
Basics of the Theory of Self-adjoint Extensions of Symmetric Operators

3.1 Deficient Subspaces and Deficiency Indices of Symmetric Operators

In this chapter, we expound only a necessary part of the general theory concerning s.a. extensions of unbounded symmetric operators, see [156, 157]. The content of this part is actually reduced to three theorems presented in Sects. 3.1, 3.3, and 3.4. These theorems are not assigned any names in the conventional mathematical literature [9, 116]; instead, their crucial formulas are called the "*von Neumann formulas*." We call these three theorems the first and second von Neumann theorems and the main theorem.[1]

We begin by recalling the minimum necessary notions and facts concerning symmetric operators from Sect. 2.7, especially Sect. 2.7.6, and introducing some new notation.

Let $\mathfrak{H}$ be a Hilbert space, and let $\hat{f}$ be a generic symmetric operator in $\mathfrak{H}$, not necessarily closed, with domain D_f and adjoint $\hat{f}^+$, $\hat{f} \subseteq \hat{f}^+$. Its closure $\overline{\hat{f}}$ with domain $D_{\overline{f}}$ is also a symmetric operator with the same adjoint, $\overline{\hat{f}} \subseteq (\overline{\hat{f}})^+ = \hat{f}^+$; we let $\underline{\xi}$ denote the vectors belonging to $D_{\overline{f}}$, $\underline{\xi} \in D_{\overline{f}}$. We let $\mathbb{C}'$ denote the set of complex numbers with nonzero imaginary parts, $\mathbb{C}' = \{z = x + iy, y \neq 0\} = \mathbb{C}_+ \cup \mathbb{C}_-$. For any $z \in \mathbb{C}'$, the range $R_{\overline{f}(z)}$ of the operator $\overline{\hat{f}}(z) = \overline{\hat{f}} - z\hat{I}$ is a closed set in $\mathfrak{H}$. The orthogonal complement of $R_{\overline{f}(z)}$ in $\mathfrak{H}$ is called the *deficient subspace* of $\hat{f}$, as well as of $\overline{\hat{f}}$, corresponding to the point $z \in \mathbb{C}'$; the deficient subspace coincides with the kernel of the operator $(\overline{\hat{f}}(z))^+ = \hat{f}^+(\overline{z}) = \hat{f}^+ - \overline{z}\hat{I}$. We let $\aleph_z$

[1]The reader interested in the final statement (without the details of a rigorous proof) can go directly to the main theorem in Sect. 3.4, and to the subsequent comments in Sect. 3.5.

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denote this deficient subspace and let $\xi_{\bar{z}}$ denote the vectors belonging to $\aleph_z$,

$$\aleph_z = R^{\perp}_{\overline{f}(z)} = \ker \hat{f}^+ (\bar{z}) = \{\xi_{\bar{z}} \in D_{f^+} : \ \hat{f}^+ \xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\}. \tag{3.1}$$

Accordingly, the decomposition

$$\mathfrak{H} = R_{\overline{f}(z)} \oplus \aleph_z \tag{3.2}$$

holds, which implies that any vector $\xi \in \mathfrak{H}$ can be represented as

$$\xi = \overline{\hat{f}}\,(z)\,\underline{\xi} + \xi_{\bar{z}}, \tag{3.3}$$

with some vectors $\underline{\xi} \in D_{\overline{f}}$ and $\xi_{\bar{z}} \in \aleph_z$ uniquely determined by ξ. We note that for a generic nonclosed operator $\hat{f}$, its closure $\overline{\hat{f}}$ enters the decompositions (3.2) and (3.3).

The dimension of the deficient subspace $\aleph_z$ is independent of z in the respective domains $\mathbb{C}_- = \{z = x + iy, \ y < 0\}$ and $\mathbb{C}_+ = \{z = x + iy, \ y > 0\}$,

$$\dim \aleph_z = \begin{cases} m_+, \ z \in \mathbb{C}_-, \\ m_-, \ z \in \mathbb{C}_+, \end{cases}$$

where m_+ and m_- are called *the deficiency indices* of the operator $\hat{f}$, as well as of $\overline{\hat{f}}$. For a given $z \in \mathbb{C}'$, we distinguish two deficient subspaces $\aleph_z$ and $\aleph_{\bar{z}}$,

$$\aleph_{\bar{z}} = \ker \hat{f}^+ (z) = \left\{\xi_z \in D_{f^+} : \ \hat{f}^+ \xi_z = z\xi_z\right\}, \tag{3.4}$$

such that if $z \in \mathbb{C}_-$ $(\mathbb{C}_+)$ then $\dim \aleph_z = m_+ \ (m_-)$, whereas[2] $\dim \aleph_{\bar{z}} = m_- \ (m_+)$. Both m_+ and m_- can be infinite. If both m_+ and m_- are infinite, they are considered equal, $m_+ = m_- = \infty$.

A basic starting point in studying symmetric operators and s.a. extensions of symmetric operators is the following theorem, which we call the *first von Neumann theorem*.

Theorem 3.1 (The first von Neumann theorem). *For any symmetric operator $\hat{f}$, the domain D_{f^+} of its adjoint $\hat{f}^+$ is the direct sum of the three subspaces $D_{\overline{f}}$, $\aleph_{\bar{z}}$, and $\aleph_z$:*

$$D_{f^+} = D_{\overline{f}} + \aleph_{\bar{z}} + \aleph_z\,, \ \forall z \in \mathbb{C}', \tag{3.5}$$

[2] We point out that there exists an anticorrespondence $z \rightleftarrows \bar{z}$ between the subscript z of $\aleph_z$ and the respective eigenvalue $\bar{z}$ and the subscript of the eigenvector $\xi_{\bar{z}}$ of $\hat{f}^+$. Perhaps it would be more convenient to change the notation $\aleph_z \rightleftarrows \aleph_{\bar{z}}$; the conventional notation is due to tradition. The same concerns the subscripts of $m_\pm$ and $\mathbb{C}_\mp$.

such that any vector $\xi_* \in D_{f^+}$ *is uniquely represented as*

$$\xi_* = \underline{\xi} + \xi_z + \xi_{\bar{z}}, \ \ \underline{\xi} \in D_{\overline{f}}, \ \xi_z \in \aleph_{\bar{z}}, \ \xi_{\bar{z}} \in \aleph_z\,, \tag{3.6}$$

and

$$\hat{f}^+ \xi_* = \overline{\hat{f}} \underline{\xi} + z\xi_z + \bar{z}\xi_{\bar{z}}\,. \tag{3.7}$$

Formula (3.6) is called the *first von Neumann formula*; we assign the same name to (3.5).

It should be emphasized that for an initial symmetric operator $\hat{f}$, the domain $D_{\overline{f}}$ of its closure $\overline{\hat{f}}$ enters the decompositions (3.5)–(3.7).

Proof. We first note that the domain $D_{\overline{f}}$ and the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are subspaces belonging to D_{f^+}; therefore, a vector $\xi_* = \underline{\xi} + \xi_z + \xi_{\bar{z}}$ belongs to D_{f^+} with any $\underline{\xi} \in D_{\overline{f}}$, $\xi_z \in \aleph_{\bar{z}}$, and $\xi_{\bar{z}} \in \aleph_z$. It remains to prove that for any vector $\xi_* \in D_{f^+}$, a unique representation (3.6) holds.

Let $\xi_* \in D_{f^+}$. According to (3.2) and (3.3), the vector $\hat{f}^+ (z)\, \xi_*$ is represented as

$$\hat{f}^+ (z)\, \xi_* = \overline{\hat{f}}(z)\underline{\xi} + (\bar{z} - z)\, \xi_{\bar{z}}\,, \ \ \forall z \in \mathbb{C}', \tag{3.8}$$

with some $\underline{\xi} \in D_{\overline{f}}$ and $\xi_{\bar{z}} \in \aleph_z$ that are uniquely determined by ξ_* (the nonzero factor $\bar{z} - z$ in front of $\xi_{\bar{z}}$ is introduced for convenience). But $\overline{\hat{f}}\underline{\xi} = \hat{f}^+\underline{\xi}$ and $\bar{z}\xi_{\bar{z}} = \hat{f}^+\xi_{\bar{z}}$, and (3.8) becomes $\hat{f}^+ (z)\, (\xi_* - \underline{\xi} - \xi_{\bar{z}}) = 0$, which yields $\xi_* - \underline{\xi} - \xi_{\bar{z}} = \xi_z$, or $\xi_* = \underline{\xi} + \xi_z + \xi_{\bar{z}}$, where ξ_z belongs to $\aleph_{\bar{z}}$ and is evidently uniquely determined by ξ_*, $\underline{\xi}$, and $\xi_{\bar{z}}$ and is therefore uniquely determined by ξ_* alone. This proves the representation (3.6) for any vector $\xi_* \in D_{f^+}$. After this representation has been established, (3.7) becomes evident. $\square$

We note that:

(a) Representations (3.5)–(3.7) hold for any $z \in \mathbb{C}'$.
(b) Although representations (3.6) and (3.7) are explicitly z-dependent, because the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$, and hence the sum[3] $\aleph_{\bar{z}} + \aleph_z$, depend on z, the subspace D_{f^+} and the operator f^+ do not depend on z, and $\dim(\aleph_{\bar{z}} + \aleph_z) = m_+ + m_-$, as well as $m_\pm$ by themselves, is independent of z.
(c) The sum in (3.5) is direct, but not orthogonal; it cannot be orthogonal because $\overline{D_{\overline{f}}} = \mathfrak{H}$, and therefore $D_{\overline{f}}^\perp = \{0\}$.

It follows immediately from the first von Neumann theorem that a nonclosed symmetric operator $\hat{f}$ is essentially s.a., and a closed symmetric operator is s.a., iff

[3] Although $\aleph_{\bar{z}}$ and $\aleph_z$ are closed subspaces in $\mathfrak{H}$, we cannot generally assert that their direct sum $\aleph_{\bar{z}} + \aleph_z$ is also a closed subspace. The latter is always true if one of the subspaces is finite-dimensional.

$\aleph_{\overline{z}} = \aleph_z = \{0\}$, i.e., iff its deficiency indices are equal to zero, $m_\pm = 0$, because in this case, $D_{f^+} = D_{\overline{f}}$, and therefore $\overline{\hat{f}} = \hat{f}^+$. In other words, the adjoint $\hat{f}^+$ is symmetric iff $m_\pm = 0$; compare with Lemma 2.75. But this theorem, namely (3.6) and (3.7), also allows estimating the asymmetricity of the adjoint $\hat{f}^+$ in the case that the deficiency indices m_+ and m_- are not equal to zero (one or both of them) and analyzing the possibilities of symmetric and s.a. extensions of $\hat{f}$. We now turn to this case, the case of $\max m_\pm \neq 0$.

3.2 Asymmetry Forms

The following consideration deals with some arbitrary, but fixed, complex number $z \in \mathbb{C}'$. A choice of a specific z is a matter of convenience, all z being equivalent; in the mathematical literature, it is a tradition to choose $z = i$.

By definition (see Sect. 2.7), a symmetric operator $\hat{f}$ is a densely defined operator satisfying the condition

$$\left(\eta, \hat{f}\xi\right) - \left(\hat{f}\eta, \xi\right) = 0, \ \forall \xi, \eta \in D_f.$$

The criterion for symmetricity of a densely defined operator $\hat{f}$ is that all its diagonal matrix elements be real-valued,[4] i.e.,

$$\left(\xi, \hat{f}\xi\right) - \left(\hat{f}\xi, \xi\right) = \left(\xi, \hat{f}\xi\right) - \overline{\left(\xi, \hat{f}\xi\right)} = 2i\,\mathrm{Im}\left(\xi, \hat{f}\xi\right) = 0\,, \ \forall \xi \in D_f;$$

see Lemma 2.50. For this reason, it is natural to introduce two forms defined by the adjoint operator $\hat{f}^+$ on its domain D_{f^+}: the sesquilinear form $\omega_{f^+}(\eta_*, \xi_*)$, given by

$$\omega_{f^+}(\eta_*, \xi_*) = \left(\eta_*, \hat{f}^+\xi_*\right) - \left(\hat{f}^+\eta_*, \xi_*\right), \ \xi_*, \eta_* \in D_{f^+}, \tag{3.9}$$

and the quadratic form $\Delta_{f^+}(\xi_*)$, which is a restriction of $\omega_{f^+}(\eta_*, \xi_*)$ to the diagonal $\xi_* = \eta_*$,

$$\Delta_{f^+}(\xi_*) = \omega_{f^+}(\xi_*, \xi_*) = 2i\,\mathrm{Im}\left(\xi_*, \hat{f}^+\xi_*\right), \ \xi_* \in D_{f^+}. \tag{3.10}$$

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[4]This is well known to physicists as applied to s.a. operators.

The form ω_{f^+} is anti-Hermitian, while the form Δ_{f^+} is pure imaginary:

$$\omega_{f^+}(\eta_*, \xi_*) = -\overline{\omega_{f^+}(\xi_*, \eta_*)}\,, \quad \overline{\Delta_{f^+}(\xi_*)} = -\Delta_{f^+}(\xi_*).$$

The form ω_{f^+} is completely determined by Δ_{f^+} in view of the equality

$$\begin{aligned}\omega_{f^+}(\eta_*, \xi_*) =& \frac{1}{4}\Big\{\left[\Delta_{f^+}(\xi_* + \eta_*) - \Delta_{f^+}(\xi_* - \eta_*)\right] \\ &- i\left[\Delta_{f^+}(\xi_* + i\eta_*) - \Delta_{f^+}(\xi_* - i\eta_*)\right]\Big\},\end{aligned}$$

which is the so-called polarization formula.

Each of these forms is a measure of asymmetricity of the adjoint operator $\hat{f}^+$, i.e., a measure of the extent to which the adjoint operator $\hat{f}^+$ deviates from a symmetric operator. We therefore call ω_{f^+} and Δ_{f^+} respectively the *sesquilinear asymmetry form* and *quadratic asymmetry form*. If $\omega_{f^+} = 0$, or equivalently, $\Delta_{f^+} = 0$, then the adjoint $\hat{f}^+$ is symmetric and $\hat{f}$ is essentially s.a.

One of the immediate advantages of introducing the sesquilinear form ω_{f^+} is that it allows simply evaluating the closure $\overline{\hat{f}}$ of an initial, generally nonclosed, symmetric operator $\hat{f}$ once the adjoint $\hat{f}^+$ is known. Indeed, by Lemma 2.43, the closure $\overline{\hat{f}}$ of a symmetric operator $\hat{f}$ can be determined as the adjoint of the adjoint, $\overline{\hat{f}} = (\hat{f}^+)^+$. The defining equation (see Sect. 2.6.1) for $(\hat{f}^+)^+ = \overline{\hat{f}}$, i.e., for pairs $\underline{\psi} \in D_{\overline{f}}$ and $\underline{\chi} = \overline{\hat{f}}\underline{\psi}$, is given by

$$\left(\underline{\psi}, \hat{f}^+\xi_*\right) - \left(\underline{\chi}, \xi_*\right) = 0\,, \ \forall \xi_* \in D_{f^+}. \tag{3.11}$$

But the inclusion $\overline{\hat{f}} \subseteq \hat{f}^+$ implies that $D_{\overline{f}} \subseteq D_{f^+}$, i.e., $\underline{\psi} \in D_{f^+}$, and $\underline{\chi} = \overline{\hat{f}}\underline{\psi} = \hat{f}^+\underline{\psi}$ (we know the "rule" for $\overline{\hat{f}}$); therefore, the defining equation (3.11) for the closure $\overline{\hat{f}}$ reduces to the equation

$$\begin{aligned}&\left(\underline{\psi}, \hat{f}^+\xi_*\right) - \left(\hat{f}^+\underline{\psi}, \xi_*\right) = \omega_{f^+}\left(\underline{\psi}, \xi_*\right) = 0 \\ &\Longrightarrow \omega_{f^+}\left(\xi_*, \underline{\psi}\right) = 0\,, \ \forall \xi_* \in D_{f^+},\end{aligned} \tag{3.12}$$

for $\underline{\psi} \in D_{\overline{f}}$ only, which is the linear equation for the domain $D_{\overline{f}} \subseteq D_{f^+}$ of the closure. The closure $\overline{\hat{f}}$ of a symmetric operator $\hat{f}$, $\hat{f} \subseteq \hat{f}^+$, is thus given by

$$\overline{\hat{f}} : \begin{cases} D_{\overline{f}} = \left\{\underline{\psi} : \underline{\psi} \in D_{f^+};\ \omega_{f^+}\left(\xi_*, \underline{\psi}\right) = 0\,, \ \forall \xi_* \in D_{f^+}\right\}, \\ \overline{\hat{f}}\underline{\psi} = \hat{f}^+\underline{\psi}\,. \end{cases} \tag{3.13}$$

Formula (3.13) specifies the closure $\overline{\hat{f}}$ of a symmetric operator $\hat{f}$ as an evidently symmetric restriction of its adjoint $\hat{f}^{+}$: the equality $\omega_{f+}\left(\xi_{*}, \underline{\psi}\right) = 0$ implies that

$$\omega_{f+}\left(\underline{\eta}, \underline{\xi}\right) = \left(\underline{\eta}, \overline{\hat{f}}\underline{\xi}\right) - \left(\overline{\hat{f}}\underline{\eta}, \underline{\xi}\right) = 0\,,\ \forall \underline{\eta}, \underline{\xi} \in D_{\overline{f}} \subseteq D_{f+}. \tag{3.14}$$

Because ω_{f+} vanishes on $D_{\overline{f}}$, and because of the representation (3.6) for $\xi_{*} \in D_{f+}$, the nontrivial content of (3.12) for the domain $D_{\overline{f}}$ in (3.13) is due only to the presence of the deficient subspaces. Indeed, substituting representation (3.6) into (3.12) and using (3.14), we reduce this equation to the equation

$$\omega_{f+}\left(\xi_{z} + \xi_{\overline{z}}, \underline{\psi}\right) = 0\,,\ \forall \xi_{z} \in \aleph_{\overline{z}}\,,\ \forall \xi_{\overline{z}} \in \aleph_{z}\,,$$

which is equivalent to

$$\omega_{f+}\left(\xi_{z}, \underline{\psi}\right) = 0\,,\ \omega_{f+}\left(\xi_{\overline{z}}, \underline{\psi}\right) = 0\,,\ \forall \xi_{z} \in \aleph_{\overline{z}}\,,\ \forall \xi_{\overline{z}} \in \aleph_{z}\,. \tag{3.15}$$

Let the deficient subspaces be finite-dimensional, $\dim \aleph_{\overline{z}} = m(\overline{z}) < \infty$ and $\dim \aleph_{z} = m(z) < \infty$ ($m(\overline{z})$ is equal to m_{+} or m_{-} and $m(z) = m_{-}$ or m_{+} for the respective $z \in \mathbb{C}_{+}$ or $z \in \mathbb{C}_{-}$), and let $\{e_{z,k}\}_{1}^{m(\overline{z})}$ and $\{e_{\overline{z},k}\}_{1}^{m(z)}$ be some bases in the respective $\aleph_{\overline{z}}$ and $\aleph_{z}$. Then the last set of equations can be replaced by a finite set of equations

$$\omega_{f+}\left(e_{z,k}, \underline{\psi}\right) = 0\,,\ \omega_{f+}\left(e_{\overline{z},l}, \underline{\psi}\right) = 0,\ k = 1, \ldots, m(\overline{z}),\ l = 1, \ldots, m(z)\,.$$

The inverse statement also holds: if

$$\omega_{f+}\left(\xi_{z}, \psi\right) = \omega_{f+}\left(\xi_{\overline{z}}, \psi\right) = 0,\ \psi \in D_{f+},\ \forall \xi_{z} \in \aleph_{\overline{z}}\,,\ \forall \xi_{\overline{z}} \in \aleph_{z},$$

then $\psi = \underline{\psi} \in D_{\overline{f}}$.

Taking the aforementioned into account, we can specify $D_{\overline{f}}$ in (3.13) as follows:

$$\begin{aligned} D_{\overline{f}} = \Big\{ & \underline{\psi} : \underline{\psi} \in D_{f+};\ \omega_{f+}\left(\xi_{z}, \underline{\psi}\right) = \omega_{f+}\left(\xi_{\overline{z}}, \underline{\psi}\right) = 0, \\ & \forall \xi_{z} \in \aleph_{\overline{z}}\,,\ \forall \xi_{\overline{z}} \in \aleph_{z} \Big\}, \end{aligned} \tag{3.16}$$

which is equivalent to

$$\begin{aligned} D_{\overline{f}} = \Big\{ & \underline{\psi} \in D_{f+} : \omega_{f+}\left(e_{z,k}, \underline{\psi}\right) = \omega_{f+}\left(e_{\overline{z},l}, \underline{\psi}\right) = 0, \\ & k = 1, \ldots, m(\overline{z})\,,\ l = 1, \ldots, m(z) \Big\}, \end{aligned} \tag{3.17}$$

in the case of finite-dimensional deficient subspaces.

3.3 Symmetric Extensions

The main advantage of the two asymmetry forms ω_{f^+} and Δ_{f^+} is that they allow a comparatively simple analysis of the possibilities of symmetric and s.a. extensions of symmetric operators and an efficient description of such extensions. The key ideas formulated, so to speak, in advance are as follows. Any symmetric extension of a symmetric operator $\hat{f}$ is simultaneously a restriction of its adjoint $\hat{f}^+$ to a subdomain in D_{f^+} such that the restriction of ω_{f^+} and Δ_{f^+} to this subdomain vanishes. On the other hand, ω_{f^+} allows a comparatively simple evaluation of the adjoint of the extension, while Δ_{f^+} allows estimating the measure of closedness of the extension and the possibility of any further extension. Because any s.a. operator does not allow nontrivial symmetric extensions, see Lemma 2.64, any s.a. extension of a symmetric operator $\hat{f}$, if it is possible, is a maximal symmetric extension. By a *maximal symmetric extension*, we mean an extension to a maximal subdomain in D_{f^+} on which ω_{f^+} and Δ_{f^+} vanish, maximal in the sense that any further extension to a larger domain on which ω_{f^+} and Δ_{f^+} vanish is impossible.

According to (3.15), both ω_{f^+} and Δ_{f^+} vanish on the domain $D_{\overline{f}} \subset D_{f^+}$ of the closure $\overline{\hat{f}} \subset \hat{f}^+$,

$$\omega_{f^+}\left(\underline{\eta}, \underline{\xi}\right) = 0\,,\ \forall \underline{\eta}, \underline{\xi} \in D_{\overline{f}} \iff \Delta_{f^+}\left(\underline{\xi}\right) = 0\,,\ \forall \underline{\xi} \in D_{\overline{f}}\,,$$

and are nonzero only because of the presence of the deficient subspaces $\aleph_{\overline{z}}$ and $\aleph_z$ (we recall that we consider the case in which $\max m_\pm \neq 0$ and at least one of the deficient subspaces is nontrivial).

Based on the first von Neumann theorem, we evaluate the contributions of the deficient subspaces to the form ω_{f^+}. Substituting representation (3.6) for both ξ_* and η_* into $\omega_{f^+}(\eta_*, \xi_*)$, then using the sesquilinearity and anti-Hermiticity of the form ω_{f^+} together with (3.14) and (3.15), we obtain that $\omega_{f^+}(\eta_*, \xi_*) = \omega_{f^+}(\eta_z + \eta_{\overline{z}}, \xi_z + \xi_{\overline{z}})$. Using now definitions (3.9), (3.1), and (3.4), we obtain the required representation of the form ω_{f^+} in terms of the deficient subspaces:

$$\omega_{f^+}(\eta_*, \xi_*) = 2iy\left[(\eta_z, \xi_z) - (\eta_{\overline{z}}, \xi_{\overline{z}})\right]\,,\ 2iy = (z - \overline{z}). \tag{3.18}$$

There follows a similar representation for the form Δ_{f^+}:

$$\Delta_{f^+}(\xi_*) = 2iy\left(\|\xi_z\|^2 - \|\xi_{\overline{z}}\|^2\right). \tag{3.19}$$

Formula (3.19) is sometimes called *the von Neumann formula* (without any number attached to it). We assign the same name to (3.18).

We can see that the asymmetricity of the adjoint operator $\hat{f}^+$ is indeed due to the deficient subspaces, and what is more, the forms ω_{f^+} and Δ_{f^+} are of a specific structure: up to a nonzero factor $(z - \overline{z}) = 2iy$, the contributions of the different deficient subspaces $\aleph_{\overline{z}}$ and $\aleph_z$ are of opposite signs, and in principle, can compensate each other under an appropriate correspondence between ξ_z and $\xi_{\overline{z}}$, which are the respective $\aleph_{\overline{z}}$- and $\aleph_z$-components of vectors $\xi_* \in D_{f^+}$.

In the present exposition, (3.18) and (3.19), together with the first von Neumann theorem, form a basis for estimating the possibility of s.a. extensions of a generic symmetric operator $\hat{f}$ and constructing all its possible s.a. extensions. Even though the forms ω_{f^+} and Δ_{f^+} and the respective formulas (3.18) and (3.19) are equivalent, it is convenient to use them both, one or another, depending on the context.

An alternative method for the study and construction of symmetric and s.a. extensions of symmetric operators is based on the so-called Cayley transformation of a closed symmetric operator $\hat{f}$ to an isometric operator $\hat{V} = \hat{f}(z)(\hat{f}(\overline{z}))^{-1}$ with domain $D_V = R_{f(\overline{z})}$ and range $R_V = R_{f(z)}$ and inverse transformation $\hat{f} = (z\hat{I} - \overline{z}\hat{V})(\hat{I} - \hat{V})^{-1}$; for reference, see [9, 116].

A nontrivial symmetric extension $\hat{f}_{\mathfrak{e}}$ of a symmetric operator $\hat{f}$, $\overline{\hat{f}} \subset \hat{f}_{\mathfrak{e}} \subseteq \hat{f}_{\mathfrak{e}}^+ \subset \hat{f}^+$, with domain $D_{f_{\mathfrak{e}}}$, $D_{\overline{f}} \subset D_{f_{\mathfrak{e}}} \subset D_{f^+}$, is possible only at the expense of the deficient subspaces $\aleph_{\overline{z}}$ and $\aleph_z$:

$$D_{f_{\mathfrak{e}}} = \left\{\xi_{\mathfrak{e}} : \xi_{\mathfrak{e}} = \underline{\xi} + \xi_{z,\mathfrak{e}} + \xi_{,\mathfrak{e}},\ \forall \underline{\xi} \in D_{\overline{f}},\ \xi_{z,\mathfrak{e}} \in \aleph_{\overline{z}},\ \xi_{\overline{z},\mathfrak{e}} \in \aleph_z\right\}$$

(any $\underline{\xi} \in D_{\overline{f}}$ and some $\xi_{z,\mathfrak{e}} \in \aleph_{\overline{z}}$ and $\xi_{\overline{z},\mathfrak{e}} \in \aleph_z$), or

$$D_{f_{\mathfrak{e}}} = D_{\overline{f}} + D_{f_{\mathfrak{e}}}^{\aleph},\ D_{f_{\mathfrak{e}}}^{\aleph} = \left\{\xi_{\mathfrak{e}}^{\aleph}\right\} \subset \aleph_{\overline{z}} + \aleph_z\,,\ \ \xi_{\mathfrak{e}}^{\aleph} = \xi_{z,\mathfrak{e}} + \xi_{\overline{z},\mathfrak{e}},$$

where the set $D_{f_{\mathfrak{e}}}^{\aleph}$ is a nontrivial one, $D_{f_{\mathfrak{e}}}^{\aleph} \neq \{0\}$.

The set $D_{f_{\mathfrak{e}}}^{\aleph}$ is a subspace, as is $D_{f_{\mathfrak{e}}}$; therefore, the sets

$$D_{\overline{z},\mathfrak{e}}^{\aleph} = \{\xi_{z,\mathfrak{e}}\} \subseteq \aleph_{\overline{z}},\ \ D_{z,\mathfrak{e}}^{\aleph} = \{\xi_{\overline{z},\mathfrak{e}}\} \subseteq \aleph_z$$

of $\xi_{z,\mathfrak{e}}$ and $\xi_{\overline{z},\mathfrak{e}}$ involved must also be certain subspaces. We only note that it is not to be supposed that $D_{f_{\mathfrak{e}}}^{\aleph}$, which is a subspace in $\aleph_{\overline{z}} + \aleph_z$, is a direct sum of $D_{\overline{z},\mathfrak{e}}^{\aleph}$ and $D_{z,\mathfrak{e}}^{\aleph}$, $D_{f_{\mathfrak{e}}}^{\aleph} \neq D_{\overline{z},\mathfrak{e}}^{\aleph} + D_{z,\mathfrak{e}}^{\aleph}$; see below.

A crucial remark here is that a symmetric extension $\hat{f}_{\mathfrak{e}}$ of $\hat{f}$ to $D_{f_{\mathfrak{e}}} = D_{\overline{f}} + D_{f_{\mathfrak{e}}}^{\aleph}$ is simultaneously a symmetric restriction of the adjoint $\hat{f}^+$ to $D_{f_{\mathfrak{e}}} \subset D_{f^+}$. In particular, this implies that we know the "rule" for $\hat{f}_{\mathfrak{e}}$; according to (3.7), $\hat{f}_{\mathfrak{e}}$ acts as $\overline{\hat{f}}$ on $D_{\overline{f}}$ and as a multiplication by z on $D_{\overline{z},\mathfrak{e}}^{\aleph}$ and by $\overline{z}$ on $D_{z,\mathfrak{e}}^{\aleph}$.

The requirement that the restriction $\hat{f}_{\mathfrak{e}}$ of the adjoint $\hat{f}^+$ to a subspace $D_{f_{\mathfrak{e}}} \subset D_{f^+}$ be symmetric is equivalent to the requirement that the restrictions of the asymmetry forms ω_{f^+} and Δ_{f^+} to $D_{f_{\mathfrak{e}}}$ vanish:

$$\omega_{f^+}(\eta_{\mathfrak{e}}, \xi_{\mathfrak{e}}) = 0,\ \forall \eta_{\mathfrak{e}},\ \xi_{\mathfrak{e}} \in D_{f_{\mathfrak{e}}};\ \Delta_{f^+}(\xi_{\mathfrak{e}}) = 0,\ \forall \xi_{\mathfrak{e}} \in D_{f_{\mathfrak{e}}}. \tag{3.20}$$

We now establish necessary and sufficient conditions for the existence of such nontrivial domains $D_{f_\mathfrak{e}}$ and describe their structure.

The conditions (3.20) are equivalent to each other. In the following consideration, we mainly deal with the quadratic asymmetry form Δ_{f+}.

According to von Neumann formula (3.19), the only nontrivial point in the condition $\Delta_{f+}(\xi_\mathfrak{e}) = 0$ is that the restriction of Δ_{f+} to $D^{\aleph}_{f_\mathfrak{e}}$ vanishes:

$$\Delta_{f+}\left(\xi^{\aleph}_\mathfrak{e}\right) = 2iy\left(\|\xi_{z,\mathfrak{e}}\|^2 - \|\xi_{\bar{z},\mathfrak{e}}\|^2\right) = 0,\ \forall \xi^{\aleph}_\mathfrak{e} \in D^{\aleph}_{f_\mathfrak{e}}. \tag{3.21}$$

It follows immediately that if one of the deficient subspaces of the initial symmetric operator $\hat{f}$ is trivial, i.e., if $\aleph_{\bar{z}} = \{0\}$ or $\aleph_z = \{0\}$, whereas the other is not, $\aleph_z \neq \{0\}$ or $\aleph_{\bar{z}} \neq \{0\}$, or equivalently, if one of the deficiency indices is equal to zero, i.e., $\min m_\pm = 0$, whereas the other is not, i.e., $\max m_\pm \neq 0$, then there are no nontrivial symmetric extensions of this operator. In other words, a symmetric operator $\hat{f}$ with $\min m_\pm = 0$ and $\max m_\pm \neq 0$ is an essentially maximal symmetric operator.

In what follows, we therefore examine the case that both of the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ of a symmetric operator $\hat{f}$ are nontrivial, or $\min m_\pm \neq 0$. We show that in this case, nontrivial symmetric extensions of $\hat{f}$ exist, and their structure can be constructively specified. Without loss of generality, we assume that

$$0 < \min m_\pm = \dim \aleph_{\bar{z}} \leq \dim \aleph_z = \max m_\pm\,,$$

which always can be achieved by an appropriate choice of z.

We first assume the existence of a nontrivial symmetric extension $\hat{f}_\mathfrak{e}$ in the case under consideration. The equation (3.21) suggests that both deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ must be involved in this extension, i.e., both $D^{\aleph}_{\bar{z},\mathfrak{e}} \neq \{0\}$ and $D^{\aleph}_{z,\mathfrak{e}} \neq \{0\}$, and any involved $\xi_{z,\mathfrak{e}} \in D^{\aleph}_{\bar{z},\mathfrak{e}} \subseteq \aleph_{\bar{z}}$ must be assigned a certain $\xi_{\bar{z},\mathfrak{e}} \in D^{\aleph}_{z,\mathfrak{e}} \subseteq \aleph_z$ of the same norm, $\|\xi_{z,\mathfrak{e}}\| = \|\xi_{\bar{z},\mathfrak{e}}\|$, for their contributions to Δ_{f+} to compensate each other. This assignment must be a one-to-one correspondence. Indeed, if, for instance, both vectors $\xi^{\aleph}_\mathfrak{e} = \xi_{z,\mathfrak{e}} + \xi_{\bar{z},\mathfrak{e}}$ and $\xi^{\aleph\prime}_\mathfrak{e} = \xi_{z,\mathfrak{e}} + \xi'_{\bar{z},\mathfrak{e}}$ belong to $D^{\aleph}_{f_\mathfrak{e}}$, then their difference $\xi^{\aleph\prime}_\mathfrak{e} - \xi^{\aleph}_\mathfrak{e} = \xi'_{\bar{z},\mathfrak{e}} - \xi_{\bar{z},\mathfrak{e}}$ with a zero $\aleph_{\bar{z}}$-component also belongs to $D^{\aleph}_{f_\mathfrak{e}}$ because $D^{\aleph}_{f_\mathfrak{e}}$ is a subspace. But (3.21) then implies that $\left\|\xi'_{\bar{z},\mathfrak{e}} - \xi_{\bar{z},\mathfrak{e}}\right\| = 0$, i.e., $\xi'_{\bar{z},\mathfrak{e}} = \xi_{\bar{z},\mathfrak{e}}$. A similar analysis for a pair of vectors $\xi^{\aleph}_\mathfrak{e} = \xi_{z,\mathfrak{e}} + \xi_{\bar{z},\mathfrak{e}} \in D^{\aleph}_{f_\mathfrak{e}}$ and $\xi^{\aleph\prime}_\mathfrak{e} = \xi'_{z,\mathfrak{e}} + \xi_{\bar{z},\mathfrak{e}} \in D^{\aleph}_{f_\mathfrak{e}}$ results in the conclusion that the equality $\xi'_{z,\mathfrak{e}} = \xi_{z,\mathfrak{e}}$ must hold. This proves that there is a one-to-one isometric correspondence between $D^{\aleph}_{\bar{z},\mathfrak{e}}$ and $D^{\aleph}_{z,\mathfrak{e}}$. Moreover, this correspondence must be a linear mapping of $D^{\aleph}_{\bar{z},\mathfrak{e}}$ onto $D^{\aleph}_{z,\mathfrak{e}}$ in order that $D^{\aleph}_{f_\mathfrak{e}}$ be a subspace.[5]

[5]We can omit this requirement because an isometric operator is linear [9].

We thus obtain that any nontrivial symmetric extension $\hat{f}_{\mathfrak{e}}$ of a symmetric operator $\hat{f}$ is determined by a certain linear isometric mapping, or simply an isometry, $\hat{U} : \aleph_{\bar{z}} \longrightarrow \aleph_z$ with domain D_U and range R_U such that

$$D_U = D^{\aleph}_{\bar{z},\mathfrak{e}} \subseteq \aleph_{\bar{z}}, \;\; R_U = D^{\aleph}_{z,\mathfrak{e}} = \hat{U} D^{\aleph}_{\bar{z},\mathfrak{e}} \subseteq \aleph_z .$$

Because any isometry preserves dimension, $D^{\aleph}_{\bar{z},\mathfrak{e}}$ and $D^{\aleph}_{z,\mathfrak{e}}$ must be of the same dimension:

$$\dim D^{\aleph}_{\bar{z},\mathfrak{e}} = \dim D^{\aleph}_{z,\mathfrak{e}} = m_U \leq \min m_{\pm} ;$$

$D^{\aleph}_{f_{\mathfrak{e}}}$ is also of dimension m_U because of the one-to-one correspondence between the $\xi_{\bar{z},\mathfrak{e}}$ and $\xi_{z,\mathfrak{e}}$ components of any vector $\xi^{\aleph}_{\mathfrak{e}} = \xi_{z,\mathfrak{e}} + \xi_{\bar{z},\mathfrak{e}} \in D^{\aleph}_{f_{\mathfrak{e}}}$. It is now reasonable to change the notation: we let D_U denote $D^{\aleph}_{\bar{z},\mathfrak{e}}$, let $\hat{U} D_U$ denote $D^{\aleph}_{z,\mathfrak{e}}$, and change the subscript "$\mathfrak{e}$" to the subscript "U" in other cases, so that $\hat{f}_{\mathfrak{e}}$, $D_{f_{\mathfrak{e}}}$, $D^{\aleph}_{f_{\mathfrak{e}}}$, etc., are now denoted by $\hat{f}_U$, D_{f_U}, $D^{\aleph}_{f_U}$, etc. In particular, D_{f_U} is now represented as follows:

$$\begin{aligned} D_{f_U} &= D_{\overline{f}} + D^{\aleph}_{f_U} = \left\{ \xi_U = \underline{\xi} + \xi^{\aleph}_U, \; \forall \underline{\xi} \in D_{\overline{f}}\,, \; \forall \xi^{\aleph}_U \in D^{\aleph}_{f_U} \right\}, \\ D^{\aleph}_{f_U} &= \left(D_U + \hat{U} D_U \right) = \left\{ \xi^{\aleph}_U = \xi_{z,U} + \xi_{\bar{z},U} \; = \xi_{z,U} + \hat{U} \xi_{z,U}\,, \right. \\ &\qquad \left. \xi_{z,U} \in D_U \subseteq \aleph_{\bar{z}}\,, \; \xi_{\bar{z},U} = \hat{U} \xi_{z,U} \in \hat{U} D_U \subseteq \aleph_z \right\}, \end{aligned} \tag{3.22}$$

where $\left(D_U + \hat{U} D_U \right)$ denotes a special subspace of dimension m_U in the direct sum $\aleph_{\bar{z}} + \aleph_z$. This subspace can be considered the "diagonal" of the direct sum $D_U + \hat{U} D_U$.

We can now prove the existence of nontrivial symmetric extensions of a symmetric operator $\hat{f}$ with $\min m_{\pm} \neq 0$ by reversing the above consideration. Namely, it is now evident that if the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ of $\hat{f}$ are nontrivial, then any isometry $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ with domain $D_U \subseteq \aleph_{\bar{z}}$ and range $\hat{U} D_U \subseteq \aleph_z$ generates a nontrivial symmetric extension $\hat{f}_U$ of $\hat{f}$ as the restriction of the adjoint $\hat{f}^+$ to the domain D_{f_U} given by (3.22) because this restriction is evidently symmetric.

We summarize the aforesaid in a theorem which we call the *second von Neumann theorem.*

Theorem 3.2 (The second von Neumann theorem). *A symmetric operator $\hat{f}$ is essentially s.a. iff its deficiency indices are equal to zero, $m_{\pm} = 0$. A symmetric operator $\hat{f}$ is essentially maximal, i.e., does not allow nontrivial symmetric, much less s.a., extensions iff one of its deficiency indices is equal to zero,* $\min m_{\pm} = 0$, *while the other is nonzero,* $\max m_{\pm} \neq 0$.

If $\min m_{\pm} \neq 0$, *i.e., both deficient subspaces* $\aleph_{\bar{z}}$ *and* $\aleph_z$ *of a symmetric operator* $\hat{f}$ *are nonzero, then nontrivial symmetric extensions of* $\hat{f}$ *exist. Any symmetric extension* $\hat{f}_U$ *of* $\hat{f}$ *is determined by some isometric operator* $\hat{U}$ *with domain* $D_U \subseteq \aleph_{\bar{z}}$ *and range* $\hat{U} D_U \subseteq \aleph_z$. *This extension is given by*

$$D_{f_U} = D_{\underline{f}} + \left(\hat{I} + \hat{U}\right) D_U = \Big\{\xi_U : \xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U}\,;$$

$$\forall \underline{\xi} \in D_{\overline{f}}\,, \forall \xi_{z,U} \in D_U \subseteq \aleph_{\bar{z}}\,,; \hat{U}\xi_{z,U} \in \hat{U} D_U \subseteq \aleph_z\Big\}, \tag{3.23}$$

and

$$\hat{f}_U \xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_{z,U} + \bar{z}\hat{U}\xi_{z,U}. \tag{3.24}$$

Conversely, any isometric operator $\hat{U} : \aleph_{\bar{z}} \longrightarrow \aleph_z$ *with domain* $D_U \subseteq \aleph_{\bar{z}}$ *and range* $\hat{U} D_U \subseteq \aleph_z$ *defines a symmetric extension* $\hat{f}_U$ *of* $\hat{f}$ *given by (3.23) and (3.24).*

The equality

$$\xi_U = \underline{\xi} + \xi_{z,U} + \hat{U}\xi_{z,U} \tag{3.25}$$

in (3.23) is called *the second von Neumann formula*.

We do not dwell on the theory of symmetric extensions of symmetric operators in every detail because it can hardly find applications in constructing QM observables; instead, we restrict ourselves to a few remarks on the general properties of arbitrary symmetric extensions. All the details can be found in [9, 116].

Remark 3.3. (i) It is evident that if $\hat{f}_U$ is a closed extension of a symmetric operator $\hat{f}$, then D_U and $\hat{U} D_U$ are closed subspaces in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$, and vice versa.

(ii) The deficient subspaces of an extension $\hat{f}_U$ are the respective subspaces

$$\aleph_{\bar{z},U} = D_U^{\perp} = \aleph_{\bar{z}} \setminus \overline{D_U} \quad \text{and} \quad \aleph_{z,U} = \left(\hat{U} D_U\right)^{\perp} = \aleph_z \setminus \overline{\hat{U} D_U},$$

the orthogonal complements of D_U and $\hat{U} D_U$ in the respective deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ of the initial symmetric operator $\hat{f}$. The deficiency indices of the extension $\hat{f}_U$ are $m_{\pm,U} = m_{\pm} - m_U$, where $m_U = \dim D_U$. The evaluation of the deficient subspaces and deficiency indices in the particular case of a maximal symmetric extension $\hat{f}_U$ is given below. Its modification to the general case is evident.

(iii) Any symmetric operator $\hat{f}$ with both deficiency indices different from zero can be extended to a maximal or s.a. symmetric operator; see below.

(iv) The description of symmetric extensions of a symmetric operator $\hat{f}$ in terms of isometries $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ is evidently z-dependent: for a given symmetric extension of $\hat{f}$, the corresponding isometry $\hat{U}$ changes with a change of z together with the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$.

3.4 Self-adjoint Extensions

Our prime interest here is in the possibility and construction of *s.a. extensions of symmetric operators* with nonzero deficiency indices.

As we mentioned above, any s.a. extension, if at all possible, is a maximal symmetric extension that does not allow further symmetric extensions. For a maximal symmetric extension $\hat{f}_U$ of a symmetric operator $\hat{f}$ with nonzero deficiency indices, the deficient subspace $\aleph_{\bar{z}}$ must be involved in the extension as a whole,[6] i.e., $D_U = \aleph_{\bar{z}}$; otherwise, a further symmetric extension is possible by extending the isometry $\hat{U}$ to the whole of $\aleph_{\bar{z}}$. The domain of a maximal symmetric extension $\hat{f}_U$ of $\hat{f}$ is thus given by

$$\begin{aligned} D_{f_U} &= D_{\overline{f}} + (\hat{I} + \hat{U})\aleph_{\bar{z}} \\ &= \left\{\xi_U : \xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z;\ \ \forall \underline{\xi} \in D_{\overline{f}},\ \forall \xi_z \in \aleph_{\bar{z}},\ \hat{U}\xi_z \in \aleph_z\right\}, \end{aligned} \tag{3.26}$$

while $\aleph_z$ can be represented as $\aleph_z = \hat{U}\aleph_{\bar{z}} \oplus \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}$, where

$$\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \left\{\xi^{\perp}_{\bar{z},U} \in \aleph_z : \left(\xi^{\perp}_{\bar{z},U}, \hat{U}\xi_z\right) = 0\,,\ \forall \xi_z \in \aleph_{\bar{z}}\right\}$$

is the orthogonal complement of a subspace $\hat{U}\aleph_{\bar{z}} \subseteq \aleph_z$ in the deficient subspace $\aleph_z$.

We now evaluate the adjoint $\hat{f}_U^+$. Because both $\hat{f}_U$ and $\hat{f}_U^+$ are the restrictions of the adjoint operator $\hat{f}^+$, $\hat{f}_U \subseteq \hat{f}_U^+ \subset \hat{f}^+$, we can use arguments similar to those used in evaluating the closure $\overline{\hat{f}}$ of $\hat{f}$; see (3.11)–(3.13). The defining equation for $\hat{f}_U^+$ is reduced to a linear equation for the domain $D_{f_U^+} \subset D_{f^+}$, i.e., for vectors $\eta_{*U} \in D_{f_U^+}$, namely,

$$\omega_{f^+}(\xi_U, \eta_{*U}) = 0,\ \ \forall \xi_U \in D_{f_U}. \tag{3.27}$$

Let $\eta_{*U} = \underline{\eta} + \eta_z + \eta_{\bar{z}}$ be the representation (3.6) of η_{*U}, which we rewrite as

$$\eta_{*U} = \underline{\eta} + \eta_z + \hat{U}\eta_z + (\eta_{\bar{z}} - \hat{U}\eta_z) = \eta_U + (\eta_{\bar{z}} - \hat{U}\eta_z),$$

where $\eta_U \in D_{f_U}$, see (3.26), and $\eta_{\bar{z}} - \hat{U}\eta_z \in \aleph_z$. Because ω_{f^+} vanishes on D_{f_U}, (3.27) reduces to an equation for the component $\eta_{\bar{z}} - \hat{U}\eta_z \in \aleph_z$,

$$\omega_{f^+}\left(\xi_U, \eta_{\bar{z}} - \hat{U}\eta_z\right) = 0\,,\ \ \forall \xi_U \in D_{f_U}. \tag{3.28}$$

---

[6]Under our agreement that $\dim \aleph_{\bar{z}} \leq \dim \aleph_z$.

Substituting (3.26) for ξ_U into (3.28) and using representation (3.18) for ω_{f^+}, we finally obtain that $(\hat{U}\xi_z, \eta_{\bar{z}} - \hat{U}\eta_z) = 0$, $\forall \xi_z \in \aleph_{\bar{z}}$, which implies that $\eta_{\bar{z}} - \hat{U}\eta_z = \eta^{\perp}_{\bar{z},U} \in (\hat{U}\aleph_{\bar{z}})^{\perp}$. Any $\eta_{*U} \in D_{f_U^+}$ is thus represented as $\eta_{*U} = \eta_U + \eta^{\perp}_{\bar{z},U}$ with some $\eta_U \in D_{f_U}$ and $\eta^{\perp}_{\bar{z},U} \in (\hat{U}\aleph_{\bar{z}})^{\perp} \subset \aleph_z$; this representation is clearly unique.

Conversely, it is evident from the above consideration that a vector $\eta_{*U} = \eta_U + \eta^{\perp}_{\bar{z},U}$ with any $\eta_U \in D_{f_U}$ and $\eta^{\perp}_{\bar{z},U} \in (\hat{U}\aleph_{\bar{z}})^{\perp}$ satisfies the defining equation (3.27), and therefore belongs to $D_{f_U^+}$. We thus obtain that

$$
\begin{aligned}
D_{f_U^+} &= D_{f_U} + \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} \\
&= \left\{\xi_{*U} : \xi_{*U} = \xi_U + \xi^{\perp}_{\bar{z},U}\,,\ \forall \xi_U \in D_{f_U}\,,\ \forall \xi^{\perp}_{\bar{z},U} \in \left(\hat{U}\aleph_{\bar{z}}\right)^{\perp}\right\}, \\
\hat{f}_U^+ \xi_{*U} &= \hat{f}_U \xi_U + \bar{z}\xi^{\perp}_{\bar{z},U}.
\end{aligned}
$$

This result allows us to answer the main question that concerns possible s.a. extensions of symmetric operators. If the subspace $(\hat{U}\aleph_{\bar{z}})^{\perp}$ is nontrivial, $(\hat{U}\aleph_{\bar{z}})^{\perp} = \aleph_z \setminus \hat{U}\aleph_{\bar{z}} \neq \{0\}$, we have a strict inclusion $D_{f_U} \subset D_{f_U^+}$, i.e., the extension $\hat{f}_U$ is only the maximal symmetric operator and not an s.a. operator. If the subspace $(\hat{U}\aleph_{\bar{z}})^{\perp}$ is trivial, $(\hat{U}\aleph_{\bar{z}})^{\perp} = \{0\}$, we have $D_{f_U} = D_{f_U^+}$, which implies the equality $\hat{f}_U = \hat{f}_U^+$, i.e., the maximal extension $\hat{f}_U$ is an s.a. operator. We now evaluate the dimension of the subspace $(\hat{U}\aleph_{\bar{z}})^{\perp}$, which provides an evident criterion for $(\hat{U}\aleph_{\bar{z}})^{\perp}$ to be nontrivial, $\dim(\hat{U}\aleph_{\bar{z}})^{\perp} \neq 0$, or trivial, $\dim(\hat{U}\aleph_{\bar{z}})^{\perp} = 0$, and respectively, for a maximal symmetric extension $\hat{f}_U$ to be non-s.a. or s.a. It appears that $\dim(\hat{U}\aleph_{\bar{z}})^{\perp}$ is essentially determined by the deficiency indices of the initial symmetric operator.

If one of the (nontrivial) deficiency indices of the initial symmetric operator $\hat{f}$ is finite, i.e., $0 < \dim \aleph_{\bar{z}} = \min m_{\pm} < \infty$, while the other, $\dim \aleph_{\bar{z}} = \max m_{\pm}$, can be infinite, we have

$$
\dim\left(\hat{U}\aleph_{\bar{z}}\right)^{\perp} = \dim \aleph_z - \dim\left(\hat{U}\aleph_{\bar{z}}\right) = \max m_{\pm} - \min m_{\pm} = |m_+ - m_-|,
$$

where we use the equality $\dim(\hat{U}\aleph_{\bar{z}}) = \dim \aleph_{\bar{z}}$. If both deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are infinite $=$ dimensional, $m_{\pm} = \infty$, we encounter the uncertainty $\dim(\hat{U}\aleph_{\bar{z}})^{\perp} = \infty - \infty$, and a special consideration is required. The point is that in this case, the isometry $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ defining the maximal symmetric extension $\hat{f}_U$ can be an isometric mapping of the infinite-dimensional subspace $\aleph_{\bar{z}}$ both into and onto the infinite-dimensional subspace $\aleph_z$. In the case of "into," the subspace $(\hat{U}\aleph_{\bar{z}})^{\perp}$ is nontrivial, $\dim(\hat{U}\aleph_{\bar{z}})^{\perp} \neq 0$, while in the case of "onto," the subspace $(\hat{U}\aleph_{\bar{z}})^{\perp}$ is trivial, $\dim(\hat{U}\aleph_{\bar{z}})^{\perp} = 0$.

It follows that:

(a) A symmetric operator $\hat{f}$ with different deficiency indices, $m_+ \neq m_-$ (which implies that $\min m_\pm < \infty$), has no s.a. extensions. Such an operator can be extended only to a maximal symmetric operator.
(b) A symmetric operator $\hat{f}$ with equal and finite deficiency indices, $m_\pm = m < \infty$, has s.a. extensions, and what is more, any maximal symmetric extension of such an operator is s.a.
(c) A symmetric operator $\hat{f}$ with infinite deficiency indices, $m_\pm = \infty$, allows both s.a. extensions and non-s.a. extensions that are maximal symmetric operators.

Any s.a. extension $\hat{f}_U$ of $\hat{f}$ is determined by an isometric mapping $\hat{U}$ of one of the deficient subspaces, for example $\aleph_{\bar{z}}$, onto another deficient subspace, $\aleph_z$, $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$. This mapping establishes an isomorphism between the deficient subspaces. Conversely, any such isometric mapping $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ defines an s.a. extension $\hat{f}_U$ of $\hat{f}$ given by (3.23) and (3.24) with $D_U = \aleph_{\bar{z}}$ and $\hat{U} D_U = \aleph_z$.

We note that there exists another way (perhaps more informative) of establishing these results. It seems evident from (3.26), and it can be proved using arguments similar to those used in proving the first von Neumann theorem, that in our case of $\dim \aleph_{\bar{z},U} \leq \dim \aleph_{z,U}$, the deficient subspaces of the maximal symmetric extension $\hat{f}_U$ are $\aleph_{\bar{z},U} = \{0\}$ and $\aleph_{z,U} = (\hat{U}\aleph_{\bar{z}})^\perp \subseteq \aleph_z$, and its respective deficiency indices are $\dim \aleph_{\bar{z},U} = \min(m_{+U}, m_{-U}) = 0$ and

$$\dim \aleph_{z,U} = \max(m_{+U}, m_{-U}) = \dim \left(\hat{U}\aleph_{\bar{z}}\right)^\perp.$$

It then remains to evaluate $\dim(\hat{U}\aleph_{\bar{z}})^\perp$ and to refer to the above-established relation between the deficiency indices of the maximal symmetric extension and its self-adjointness: the maximal symmetric extension is s.a. iff both its deficient indices are equal to zero.

The presented consideration seems more direct.

An s.a. extension $\hat{f}_U$ of a symmetric operator $\hat{f}$ with equal deficiency indices, i.e., with isomorphic deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$, that is specified by an isometry $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ and is given by (3.23) and (3.24) with $D_U = \aleph_{\bar{z}}$ and $\hat{U} D_U = \aleph_z$ can be equivalently determined in terms of the sesquilinear asymmetry form ω_{f^+} similarly to the closure $\overline{\hat{f}}$; see (3.13) and (3.15). Namely, $\hat{f}_U$ is such an extension iff it is a restriction of the adjoint $\hat{f}^+$ to the domain D_{f_U} defined by the linear equation

$$\omega_{f^+}\left(\eta_z + \hat{U}\eta_z, \xi_U\right) = 0\,,\ \xi_U \in D_{f_U} \subset D_{f^+}\,,\ \forall \eta_z \in \aleph_{\bar{z}}\,. \tag{3.29}$$

Necessity: let $\hat{f}_U$ be an s.a. extension of $\hat{f}$. Then the restriction of the form ω_{f^+} to its domain D_{f_U} vanishes, i.e., $\omega_{f^+}(\eta_U, \xi_U) = 0$, $\forall \xi_U, \eta_U \in D_{f_U}$. Using now the representation $\eta_U = \underline{\eta} + \eta_z + \hat{U}\eta_z$ and the equality $\omega_{f^+}\left(\underline{\eta}, \xi_U\right) = 0$, see (3.12) with $\underline{\psi} = \underline{\eta}$ and $\xi_* = \xi_U$, we reduce the equality $\omega_{f+}(\eta_U, \xi_U) = 0$, $\forall \xi_U, \eta_U \in D_{f_U}$, to (3.29).

Sufficiency: let $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ be an isometry of one of the deficient subspaces onto another. We consider the linear equation (3.29) for a subspace $D_{f_U} = \{\xi_U\} \subset D_{f+}$ and show that its general solution is given by

$$\xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z \,, \ \forall \underline{\xi} \in D_{\overline{f}} \,, \ \forall \xi_z \in \aleph_{\bar{z}} \,, \ \hat{U}\xi_z \in \aleph_z \,. \tag{3.30}$$

Indeed, a vector ξ_U of the form (3.30) evidently satisfies (3.29),

$$\omega_{f+}\left(\eta_z + \hat{U}\eta_z, \underline{\xi} + \xi_z + \hat{U}\xi_z\right) = 2iy\left[(\eta_z, \xi_z) - \left(\hat{U}\eta_z, \hat{U}\xi_z\right)\right] = 0,$$

where we use (3.18) and the fact that $\hat{U}$ is an isometry. Conversely, let a vector $\xi_U \in D_{f+}$ satisfy (3.29). Using the representation

$$\xi_U = \underline{\xi} + \xi_z + \xi_{\bar{z}} = \underline{\xi} + \xi_z + \hat{U}\xi_z + \left(\xi_{\bar{z}} - \hat{U}\xi_z\right),$$

where $\underline{\xi} \in D_{\overline{f}}$, $\xi_z \in \aleph_{\bar{z}}$, $\xi_{\bar{z}}, \hat{U}\xi_z \in \aleph_z$, then using (3.18) and that $\hat{U}$ is an isometry, we reduce (3.29) to $(\hat{U}\eta_z, \xi_{\bar{z}} - \hat{U}\xi_z) = 0$, $\forall \eta_z \in \aleph_{\bar{z}}$, whence it follows that $\xi_{\bar{z}} - \hat{U}\xi_z = 0$, or $\xi_{\bar{z}} = \hat{U}\xi_z$, because $\left\{\hat{U}\eta_z, \forall \eta_z \in \aleph_{\bar{z}}\right\} = \hat{U}\aleph_{\bar{z}} = \aleph_z$.

We note that (3.29) is actually the defining equation for the adjoint $\hat{f}_U^+$ of the operator $\hat{f}_U$ that is the restriction of the adjoint operator $\hat{f}^+$ to the domain $D_{f_U} = D_{\overline{f}} + (\hat{I} + \hat{U})\aleph_{\bar{z}}$, an equation that we already encountered above, see (3.27), where the substitutions $\xi_U \to \eta_U$ and $\eta_{*U} \to \xi_U$ must be made. Its solution in the case of $\hat{U}\aleph_{\bar{z}} = \aleph_z$ shows that $\hat{f}_U^+ = \hat{f}_U$.

In the case of a symmetric operator $\hat{f}$ with equal and finite deficiency indices, $m_\pm = m < \infty$, the isometry $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$, and hence an s.a. extension $\hat{f}_U$, can be specified by a unitary $m \times m$ matrix. To this end, we choose a certain orthonormal basis $\{e_{z,k}\}_1^m$ in $\aleph_{\bar{z}}$ such that any vector $\xi_z \in \aleph_{\bar{z}}$ is represented as $\xi_z = \sum_{k=1}^m c_k e_{z,k}$, $c_k \in \mathbb{C}$, and a certain orthonormal basis $\{e_{\bar{z},l}\}_1^m$ in $\aleph_z$. Then any isometric operator $\hat{U}$ with domain $\aleph_{\bar{z}}$ and range $\aleph_z$ is given by

$$\hat{U}e_{z,k} = \sum_{k=1}^m U_{lk} e_{\bar{z},l} \,, \text{ or } \hat{U}\xi_z = \sum_{l=1}^m \left(\sum_{k=1}^m U_{lk} c_k\right) e_{\bar{z},l},$$

where $U = \{U_{lk}\}$ is a unitary matrix. Conversely, any unitary $m \times m$ matrix U defines an isometry $\hat{U}$ given by the above formulas. It is evident that for a given $\hat{U}$, the matrix U changes appropriately with the change of the orthogonal bases $\{e_{z,k}\}_1^m$ and $\{e_{\bar{z},l}\}_1^m$.

It follows that in the case under consideration, the family $\{\hat{f}_U\}$ of all s.a. extensions of a given symmetric operator $\hat{f}$ is a manifold of dimension m^2 that is a unitary group $U(m)$.

This result can be extended to the case of infinite deficiency indices, $m = \infty$.

In the case that both deficiency indices coincide, there is no difference in the choice of $z \in \mathbb{C}_+$ or $z \in \mathbb{C}_-$. In what follows, we take $z \in \mathbb{C}_+$, so from this point on, $m_+ = \dim \aleph_{\bar{z}}$ and $m_- = \dim \aleph_z$.

We now summarize all the relevant previous results in a theorem that we call the *main theorem*. This theorem is of paramount importance: it is precisely what we need from mathematics for our physical purposes. We therefore present this theorem in sufficient detail and in fact, in an independent self-contained way for the ease of using the theorem without any further references.

Theorem 3.4 (The main theorem). *Let $\hat{f}$ be an initial symmetric operator with domain D_f and adjoint $\hat{f}^+$, $\hat{f} \subseteq \hat{f}^+$, let $\aleph_{\bar{z}}$ and $\aleph_z$ be the deficient subspaces of $\hat{f}$,*

$$\aleph_{\bar{z}} = \ker \hat{f}^+(z) = \left\{\xi_z : \hat{f}^+\xi_z = z\xi_z\right\},$$

$$\aleph_z = \ker \hat{f}^+(\bar{z}) = \left\{\xi_{\bar{z}} : \hat{f}^+\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}\right\},$$

where $z \in \mathbb{C}_+$ is arbitrary, but fixed, and let $m_\pm$ be the deficiency indices of $\hat{f}$, $m_+ = \dim \aleph_{\bar{z}}$ and $m_- = \dim \aleph_z$

The operator $\hat{f}$ has s.a. extensions $\hat{f}_U = \hat{f}_U^+$, $\hat{f} \subseteq \hat{f}_U$ iff both its deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ are isomorphic, or iff its deficiency indices are equal, $m_\pm = m$.

If the deficient subspaces are trivial, i.e., if both deficiency indices are equal to zero, $m_\pm = 0$, the operator $\hat{f}$ is essentially s.a., and its unique s.a. extension is its closure $\overline{\hat{f}} = (\hat{f}^+)^+$, which coincides with its adjoint, $\overline{\hat{f}} = (\overline{\hat{f}})^+ = \hat{f}^+$.

If the deficient subspaces are nontrivial, i.e., if the deficiency indices are different from zero, $m_\pm = m \neq 0$, there exists an m^2-parameter family $\{\hat{f}_U\}$ of s.a. extensions that is the manifold $U(m)$, a unitary group.

Each s.a. extension $\hat{f}_U$ is determined by an isometric mapping $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ of one of the deficient subspaces onto another and is given by

$$\begin{aligned} D_{f_U} &= D_{\overline{f}} + \left(\hat{I} + \hat{U}\right)\aleph_{\bar{z}} \\ &= \left\{\xi_U : \xi_U = \underline{\xi} + \xi_z + \hat{U}\xi_z,\ \ \forall \underline{\xi} \in D_{\overline{f}},\ \forall \xi_z \in \aleph_{\bar{z}},\ \hat{U}\xi_z \in \aleph_z\right\}, \end{aligned} \tag{3.31}$$

where $D_{\overline{f}}$ is the domain of the closure $\overline{\hat{f}}$, and

$$\hat{f}_U\xi_U = \overline{\hat{f}}\underline{\xi} + z\xi_z + \bar{z}\hat{U}\xi_z \,. \tag{3.32}$$

Conversely, any isometry $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$ *that establishes an isomorphism between the deficient subspaces defines an s.a. extension* $\hat{f}_U$ *of* $\hat{f}$ *given by (3.31) and (3.32).*

The s.a. extension $\hat{f}_U$ *can be equivalently defined as an s.a. restriction of the adjoint* $\hat{f}^+$ *given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\xi_U : \xi_U \in D_{f^+};\ \omega_{f^+}\left(\eta_z + \hat{U}\eta_z, \xi_U\right) = 0,\ \forall \eta_z \in \aleph_{\bar{z}}\right\}, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U. \end{cases} \tag{3.33}$$

If the deficient subspaces are finite-dimensional, $0 < m < \infty$*, then s.a. extensions* $\hat{f}_U$ *can be specified in terms of unitary matrices* $U \in U(m)$*. Namely, let* $\{e_{z,k}\}_1^m$ *and* $\{e_{\bar{z},l}\}_1^m$ *be some orthogonal bases in the respective deficient subspaces* $\aleph_{\bar{z}}$ *and* $\aleph_z$*. Then an s.a. extension* $\hat{f}_U$ *is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{ \begin{array}{l} \xi_U : \xi_U = \underline{\xi} + \sum_{k=1}^m c_k e_{U,k},\ \forall \underline{\xi} \in D_{\overline{f}}, \\ \forall c_k \in \mathbb{C},\ e_{U,k} = e_{z,k} + \sum_{l=1}^m U_{lk} e_{\bar{z},l}, \end{array} \right\}, \\ \hat{f}_U \xi_U = \overline{\hat{f}} \underline{\xi} + \sum_{k=1}^m c_k \left(z e_{z,k} + \bar{z} \sum_{l=1}^m U_{lk} e_{\bar{z},l}\right), \end{cases} \tag{3.34}$$

where $U = \|U_{lk}\|$ *is a unitary matrix.*

An equivalent definition of $\hat{f}_U$ *in terms of the adjoint* $\hat{f}^+$ *becomes*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\xi_U : \xi_U \in D_{f^+};\ \omega_{f^+}(e_{U,k}, \xi_U) = 0,\ \forall k\right\}, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U. \end{cases} \tag{3.35}$$

The main theorem finishes our exposition of the general theory of s.a. extensions of symmetric operators.

3.5 Summary

We would like to finish this chapter with a comment about a possible application of the general theory of s.a. extensions of symmetric operators to the physical problem of constructing QM observables as s.a. operators, the problem that was extensively discussed in Chap. 1. We mainly address the case of nontrivial physical systems with boundaries and/or singularities of interaction where observables are represented by differential operators and where the main difficulties are related to a proper definition of s.a. Hamiltonians. Our comment has the form of brief "instructions", which are of a preliminary nature. A more detailed discussion of ordinary s.a. differential operators including their spectral analysis is given in Chaps. 4 and 5.

We recall that the challenge is to construct an s.a. operator starting from a preliminary "candidate" for a QM observable,[7] a certain formal expression giving "a rule of action" and formally s.a., in particular, starting from an s.a. differential operation[8] $\check{f}(x, -i d_x)$.

3.5.1 The First Step

The first step of a standard program for solving this problem is to give the meaning of a symmetric operator $\hat{f}$ in an appropriate Hilbert space $\mathfrak{H}$ to the formal expression by indicating its domain $D_f \subseteq \mathfrak{H}$, which must be dense. In the case of singular differential operators arising under quantization of nontrivial physical systems, this is usually achieved by choosing a domain D_f in a Hilbert space of functions (wave functions in the conventional physical terminology) like $L^2(a, b)$ so that it avoids the problems associated with boundaries and singularities. The simplest way is to require that wave functions in D_f vanish fast enough near the boundaries and singularities. The symmetricity of $\hat{f}$ is then easily verified by integrating by parts. A symmetric operator thus defined will be called an *initial symmetric operator* $\hat{f}$ in what follows; see also Chap. 5.

3.5.2 The Second Step

We then must evaluate the adjoint operator $\hat{f}^+$, i.e., find its "rule of action" and its domain $D_{f^+} \supseteq D_f$, solving the defining equation for the adjoint $\hat{f}^+$. In general, this is a nontrivial task. Fortunately, as regards differential operators, the solution of this task for rather general symmetric operators is known in the mathematical literature—see, for example, [9, 116, 128, 131, 142]—and is presented in the next chapter.

3.5.3 The Third Step

This step consists in evaluating the deficient subspaces $\aleph_{\bar{z}}$ and $\aleph_z$ with some fixed $z \in \mathbb{C}_+$ as the spaces of solutions of the respective equations $\hat{f}^+\xi_z = z\xi_z$, $\xi_z \in D_{f^+}$, and $\hat{f}^+\xi_{\bar{z}} = \bar{z}\xi_{\bar{z}}$, $\xi_{\bar{z}} \in D_{f^+}$, and in determining the deficiency indices $m_+ = \dim \aleph_{\bar{z}}$ and $m_- = \dim \aleph_z$. This problem can also present a laborious task. In the case of differential operators, it usually requires extensive experience in special functions.

[7]Provided, for example, by canonical quantization rules for classical observables $f(q, p)$.

[8]Self-adjoint by Lagrange.

Suppose the deficiency indices to have been found. If they are found to be unequal, $m_+ \neq m_-$, our work stops with the inconsolable conclusion that there is no QM analogue for the given classical observable $f(q, p)$. Such a situation, i.e., unequal deficiency indices, is encountered in physics, thus preventing some classical observables to be transferred to the quantum level (an example is the momentum of a particle on a semiaxis; see below). We note in advance that for s.a. differential operators with real coefficients, the deficiency indices are always equal.

If the deficiency indices are found to be zero, $m_\pm = 0$, our work also stops: a symmetric operator $\hat{f}$ is essentially s.a., and a uniquely defined QM observable is its closure $\overline{\hat{f}}$, which coincides with the adjoint $\hat{f}^+$, $\overline{\hat{f}} = \hat{f}^+$.

If the deficiency indices are found to be equal and nonzero, $m_\pm = m > 0$, the fourth step becomes a necessity.

3.5.4 The Fourth Step

At this step, we correctly specify the entire m^2-parameter family $\{\hat{f}_U\}$ of s.a. extensions $\hat{f}_U$ of an initial symmetric operator $\hat{f}$ in terms of isometries $\hat{U} : \aleph_{\bar{z}} \longmapsto \aleph_z$, or in terms of unitary $m \times m$ matrices U. The general theory provides two ways of specification given by the main theorem. The specification based on (3.31) and (3.32) or (3.34) (and usually presented in the mathematical literature) appears more explicit in comparison with the specification based on (3.33) or (3.35), which requires solving the corresponding linear equation for the domains D_{f_U}. But the first specification assumes knowledge of the closure $\overline{\hat{f}}$ of $\hat{f}$ if the initial symmetric operator is nonclosed,[9] which requires solving linear equations in (3.13), (3.16), or (3.17) for the domain $D_{\overline{\hat{f}}}$. The second specification can sometimes become more economical because it avoids the evaluation of the closure $\overline{\hat{f}}$ and deals directly with the domains D_{f_U} of extensions. This particularly concerns the case of differential operators where $\hat{f}^+$ is usually given by the same differential expression as the initial operator $\hat{f}$ and where the second specification allows eventually specifying the s.a. extensions $\hat{f}_U$ in the customary form of s.a. boundary conditions; an additional advantage is that only the asymptotic behavior of functions belonging the deficient subspaces near boundaries and singularities is actually required to be known. This possibility is discussed in Chap. 4. We say in advance that we also propose a third possible way of specifying s.a. extensions of symmetric differential operators directly in terms of, generally asymptotic, boundary conditions; see Chap. 4.

[9] We would like to emphasize that at this point, the general theory requires evaluating the closure $\overline{\hat{f}}$. It is precisely $\overline{\hat{f}}$ and $D_{\overline{f}}$ that enter (3.31), (3.32), (3.34), and (3.35), while in the physics literature we can sometimes see that in citing and using these formulas, $\hat{f}$ and D_f stand for $\overline{\hat{f}}$ and $D_{\overline{f}}$ even for a nonclosed symmetric operator $\hat{f}$, which is incorrect.

3.5.5 The Final Step

The final step is the standard spectral analysis, i.e., finding the spectrum and (generalized) eigenvectors of the resulting s.a. extensions $\hat{f}_U$ and their proper physical interpretation; see Chap. 5. The problem of the physical interpretation of the new m^2 parameters, which are absent from the initial formal expression and from the initial symmetric operator $\hat{f}$ and are associated with the isometries $\hat{U}$ or unitary matrices U in the case of nonzero deficiency indices, is sometimes the most difficult one. The usual approach to solving this problem is related to a search for an appropriate regularization of singularities in the operator $\hat{f}$.

The above-described general procedure for constructing QM observables starting from preliminary formal expressions is not universally obligatory. In some particular cases, more immediate procedures are possible, especially if there exist additional physical arguments. For example, in some cases, we can guess a proper domain D_f for an initial symmetric operator $\hat{f}$ such that $\hat{f}$ proves to be essentially s.a. from the very beginning.

Chapter 4
Differential Operators

The present chapter is devoted to differential operators, more specifically, to a comparative presentation of various methods of constructing s.a. differential operators starting from formal s.a. differential operations. All the constructions are based on the general theory of s.a. extensions of symmetric operators outlined in the previous chapter. They cannot, however, be considered simple applications of the general theory: they possess such additional features that make it necessary to present differential operators as a separate chapter, which reveals the specific features of differential operators, in particular, specific ways of describing s.a. extensions of various symmetric operators. The peculiarity of ordinary differential operators lies mainly in the fact that the asymmetry forms ω_{f+} and Δ_{f+} permit their representation in terms of boundary forms, which, eventually, allows one to define s.a. operators in terms of s.a. boundary conditions.

Because of a particular importance of this subject for QM, we have attempted to make the exposition of this chapter as self-contained as possible, so that the reader could read it independently of Chap. 3. With respect to Chap. 3, it is actually sufficient to be familiar with it only as far as the main theorem (Theorem 3.4) and the brief "instructions" in Sect. 3.5.

It seems useful to make some remarks concerning the subject of our exposition from the standpoint of the general theory of differential operators.

The subject area of differential operators has an almost century-long history and is inexhaustible in its volume. We restrict ourselves to ordinary differential operators in Hilbert spaces $L^2(a,b)$, scalar operators. But the main results and conclusions presented below can be extended to matrix differential operators in Hilbert spaces of vector functions such as $L^2(a,b) \oplus L^2(a,b) \oplus \cdots$ with some obvious modifications.

The foundations of the general theory of ordinary differential equations, including their spectral analysis, were laid by Weyl [161–163]. Further development of the theory, including different approaches to the subject and discussions of a number of particular questions, can be traced along [9, 27, 51, 71, 79, 80, 93, 99, 102, 108, 116, 128, 131, 132, 142, 143, 148, 156, 160]. This list of references is mainly oriented to physicists and in no way pretends to be complete; it can be considerably extended and will be continued below.

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As for partial differential operators, we refer to [24, 27, 56, 96, 99, 128, 131, 142, 149], where an extensive bibliography on the subject can be found. To physicists, we especially recommend the books [27,56], where three-dimensional Hamiltonians were classified.

We leave aside the theory of non-s.a. differential operators, which may have some applications in the physics of open systems with emission and absorption.

The problem of spectral analysis of a physically important class of s.a. differential operators is discussed in the next chapter.

4.1 Differential Operations

A linear differential operation $\check{f}$ of order $n \geq 0$ on the interval[1] (a, b) is an expression of the form

$$\check{f} = f_n(x)\, d_x^n + f_{n-1}(x)\, d_x^{n-1} + \cdots + f_1(x)\, d_x + f_0(x)\,, \tag{4.1}$$

where the functions $f_k(x)$, $k = 0, 1, \ldots, n$, defined on (a, b) are called the coefficient functions, or simply coefficients, of the differential operation. It is naturally adopted that $f_n(x) \neq 0$. A differential operation of order zero is a function.

The differential operation $\check{f}$ of (4.1) is naturally applicable to functions $\psi(x)$ that are a.c. in the interval together with their $n-1$ derivatives[2] $\psi^{(1)}, \ldots, \psi^{(n-1)}$ $\left(\psi^{(1)} = \psi'\right)$ producing differential expressions

$$\check{f}\psi(x) = \sum_{k=0}^{n} f_k(x)\, \psi^{(k)}(x)\,,$$

and generating linear differential equations, the homogeneous one $\check{f}\psi(x) = 0$ and the inhomogeneous one $\check{f}\psi(x) = \chi(x)$. Under conditions that $\psi(x)$ is square-integrable on (a, b) together with $\check{f}\psi(x)$, the differential operation $\check{f}$ generates a differential operator in the Hilbert space $L^2(a, b)$. Depending on the properties of the coefficient functions of the $\check{f}$, various additional requirements can be imposed on the functions $\psi(x)$, so that a differential operation $\check{f}$ can generate various operators in $L^2(a, b)$. All such operators are called the differential operators associated with a given differential operation. We let $\hat{f}$, with a possible subscript or/and superscript, denote a differential operator associated with a given differential operation $\check{f}$. The associated operators $\hat{f}$ differ by their domains D_f, while the "rule of action" of all the operators is given by $\check{f}$.

[1] Our conventions about understanding this notion and the related terminology are explained in Sect. 2.3.1.

[2] The derivative of order k of a function ψ is commonly denoted by $\psi^{(k)}$.

Admissible domains of operators associated with a given differential operation $\check{f}$ (4.1) depend on regularity (integrability, continuity, differentiability, etc.) of the coefficients of $\check{f}$. The standard conditions on the coefficients are that the coefficients $f_k(x)$, $k = 1, \ldots, n$, should be a.c. in the interval (a, b) together with their $k - 1$ derivatives, and their kth derivatives and the coefficient $f_0(x)$ should be locally integrable (the local integrability means (absolute) integrability in any finite interval inside (a, b)). These conditions are sufficient for the product $\chi(x)\check{f}\psi(x)$ to allow its integration by parts and for the corresponding adjoint differential operation (see below) with coefficients satisfying the same conditions to exist. The coefficients, for example $f_0(x)$, may tend to infinity as $x \to a$ and/or $x \to b$. In addition, it is required that the functions $f_k(x)/f_n(x)$, $k = 0, \ldots, n - 1$, and $1/f_n(x)$ be locally integrable. This condition is necessary for the standard theory of differential equations to be applicable to the linear differential equations generated by a given differential operation like $\check{f}\psi = 0$, $(\check{f} - W)\psi = 0$, and $\check{f}\psi = \chi$, $(\check{f} - W)\psi = \chi$, $W \in \mathbb{C}$ (as a rule, we henceforth omit the obvious function argument x). For reasons that will become clear later, we call the solutions of these equations that are a.c. in (a, b) together with their $n - 1$ derivatives the *ordinary solutions*. We do not consider here the cases in which the coefficients have nonintegrable singularities inside the interval.[3] If the singularities are located at interior points of the interval (as, for example, in the case of δ-potentials), the consideration must be appropriately modified; see in this respect Chap. 7.

A differential operation (4.1) is called a *regular differential operation* if the interval (a, b) is finite and if the functions f_k/f_n, $k = 0, \ldots, n - 1$, and $1/f_n$ are integrable on the interval (a, b), i.e., on the closed interval $[a, b]$ including the endpoints. In the opposite case, i.e., if at least one of these conditions does not hold, $\check{f}$ is called a *singular differential operation*. The left endpoint a is called a *regular endpoint* if $a > -\infty$ and the functions f_k/f_n and $1/f_n$ are integrable on a subinterval $[a, \beta]$, $\beta < b$. In the opposite case, i.e., if at least one of these conditions is invalid, the endpoint a is called a *singular endpoint*. Similar notions are introduced for the right endpoint b. For a regular differential operation, both endpoints of the interval are evidently regular.

In order to facilitate some technical points of the following exposition, we assume that the coefficient functions f_k are smooth functions in the interval (a, b) (although they can be singular at finite endpoints). We partly justify this assumption by noting that this condition holds for most QM problems. On the other hand, this assumption allows a comparatively simple proof of some of the basic assertions that hold in more general cases. We make special reservations concerning each of these cases; in particular, the standard conditions on the coefficients can be considerably weakened for even s.a. differential operations in their canonical representation (see below).

We now turn our attention to some other notions related to differential operations.

[3]This restriction is natural, e.g., for radial Hamiltonians.

Let the functions φ and ϕ belong to $\mathcal{D}(a,b)$, the space of compactly supported smooth functions; see Sect. 2.1. It is evident that $\check{f}\varphi \in \mathcal{D}(a,b)$ and $\varphi, \phi, \check{f}\varphi \in L^2(a,b)$. We consider the integral $\int_a^b \mathrm{d}x\overline{\phi}\check{f}\varphi$, which can be treated as the scalar product $\left(\phi, \check{f}\varphi\right)$ in $L^2(a,b)$,

$$\left(\phi, \check{f}\varphi\right) = \int_a^b \mathrm{d}x\overline{\phi}\check{f}\varphi = \int_a^b \mathrm{d}x \sum_{k=1}^{n} \overline{\phi} f_k \varphi^{(k)}.$$

Integrating each term $\overline{\phi} f_k \varphi^{(k)}$ by parts k times, and taking the vanishing of boundary terms into account because φ and ϕ vanish near the boundaries, we obtain

$$\left(\phi, \check{f}\varphi\right) = \int_a^b \mathrm{d}x \overline{\check{f}^*\phi}\varphi = \left(\check{f}^*\phi, \varphi\right),$$

where the differential operation $\check{f}^*$ is given by

$$\check{f}^* = (-d_x)^n \overline{f_n} + (-d_x)^{n-1} \overline{f_{n-1}} + \cdots + (-d_x)\overline{f_1} + \overline{f_0}. \tag{4.2}$$

This differential operation (4.2) is called the *adjoint differential operation*, or the *adjoint by Lagrange*, with respect to the initial differential operation $\check{f}$. The adjoint differential operation $\check{f}^*$ can be presented in the standard form (4.1),

$$\check{f}^* = \sum_{k=0}^{n} f_k^*(x)\, d_x^k, \quad f_k^*(x) = \sum_{l=0}^{n-k} (-1)^{k+l} \binom{l+k}{k} \overline{f_{k+l}^{(l)}(x)},$$

where $\binom{m}{n}$ are binomial coefficients.

A differential operation $\check{f}$ is called an *s.a. differential operation*, or *s.a. by Lagrange*, if it coincides with its adjoint, $\check{f} = \check{f}^*$. The self-adjointness of a differential operation $\check{f}$ is equivalent to the equality

$$\left(\phi, \check{f}\varphi\right) = \left(\check{f}\phi, \varphi\right), \ \forall \varphi, \phi \in \mathcal{D}(a,b). \tag{4.3}$$

We emphasize that the self-adjointness of a differential operation is only a necessary, and generally not sufficient, condition for its associated operator $\hat{f}$ in $L^2(a,b)$ to be s.a. But only s.a. differential operations that can generate s.a. differential operators are interesting from the standpoint of QM. The main problem is to indicate a proper domain in $L^2(a,b)$ for an s.a. $\check{f}$. This proves to be impossible sometimes, whereas in other cases, a family of different s.a. operators can be associated with a given s.a. differential operation.

We describe the general structure of s.a. differential operations of arbitrary order. The coefficients of an s.a. differential operation $\check{f}$ satisfy the relations

$$f_k(x) = \sum_{l=0}^{n-k} (-1)^{k+l} \binom{l+k}{k} \overline{f_{k+l}^{(l)}(x)}, \quad k = 0, 1, \ldots, n.$$

These relations can be resolved in the general form, which results in the so-called *canonical form of an s.a. differential operation*

$$\begin{aligned} \check{f} &= \sum_{l=0}^{n} \check{f}_{(l)}, \quad \check{f}_{(2k)} = (-d_x)^k \phi_{2k} d_x^k, \\ \check{f}_{(2k+1)} &= \frac{i}{2}\left[(-d_x)^{k+1} \phi_{2k+1} d_x^k + d_x^k \phi_{2k+1} (-d_x)^{k+1}\right], \\ \overline{\phi_{2k}} &= \phi_{2k}, \quad \overline{\phi_{2k+1}} = \phi_{2k+1}, \end{aligned} \tag{4.4}$$

which is a sum of even canonical s.a. differential monomials $\check{f}_{(2k)}$ of even order $2k$ with real coefficients $\phi_{2k}(x)$, $k = 0, 1, \ldots, [n/2]$, and odd canonical s.a. differential binomials $\check{f}_{(2k+1)}$ of odd order $2k+1$ with pure imaginary coefficient $i\phi_{2k+1}(x)$, $k = 0, 1, \ldots, [(n-1)/2]$.

Even s.a. differential operations of even order n, $n/2 \in \mathbb{Z}_+$, are the sum of only even s.a. monomials,

$$\begin{aligned} \check{f} &= \sum_{k=0}^{n/2} \check{f}_{(2k)} = \sum_{k=0}^{n/2} (-d_x)^k \phi_{2k} d_x^k \\ &= \sum_{k=0}^{n/2} (-d_x)^k p_{n/2-k} d_x^k, \quad p_{n/2-k} = \phi_{2k}, \end{aligned} \tag{4.5}$$

and their coefficients are real; conversely, any s.a. differential operation with real coefficients is even. *Odd s.a. differential operations* of odd order n, $(n-1)/2 \in \mathbb{Z}_+$, are the sum of only odd s.a. binomials, $\check{f} = \sum_{k=0}^{(n-1)/2} \check{f}_{(2k+1)}$, and their coefficients are pure imaginary; any s.a. differential operation with pure imaginary coefficients is odd. The general s.a. differential operation that is a sum of both even monomials and odd binomials can be called a mixed one.

The simplest odd s.a. differential operation is

$$\check{p} = -id_x, \tag{4.6}$$

and is identified with the QM momentum operator for a particle moving on an interval of the real axis;[4] see Chap. 1. This differential operation and its associated operators, in particular, possible s.a. operators, are considered in detail in Chap. 6.

The simplest even s.a. differential operation is given by

$$\check{\mathcal{H}} = -d_x^2. \tag{4.7}$$

In the physics literature, it is usually identified (for simplicity, we omit here the factor $1/2m$; see (1.5)) with the QM Hamiltonian for a free particle moving on an interval of the real axis. Its simplest modification

$$\check{H} = \check{\mathcal{H}} + V(x) = -d_x^2 + V(x), \; V(x) = \overline{V(x)}, \tag{4.8}$$

is identified with the QM Hamiltonian for a particle in a potential field $V(x)$. Such second-order differential operations with various potentials $V(x)$ and their associated s.a. operators are considered in detail in Chaps. 7–10.

Even s.a. differential operations are distinguished in a certain way. First, at least one s.a. operator is associated with any such differential operations (see below). Second, the theory of linear differential equations generated by even s.a. differential operations $\check{f}$ can be conveniently formulated in terms of the so-called quasiderivatives, which have made possible great advances in developing the theory of even s.a. differential operators associated with even s.a. differential operations; in particular, the associated s.a. operators can be conveniently specified in terms of the quasiderivatives; for details, see [9, 116]. We reproduce the corresponding definitions below.

For each even s.a. differential operation $\check{f}$ of order n, we introduce the quasiderivative differential operations $\check{K}_x^{[k]}$, $k = 1, \dots, n$, defined recursively for a given $\check{f}$ by

$$\check{K}_x^{[k]} = d_x^k, \; k = 0, \dots, n/2 - 1, \; \check{K}_x^{[n/2]} = p_0 d_x^{n/2},$$
$$\check{K}_x^{[n/2+k]} = p_k d_x^{n/2-k} - d_x \check{K}_x^{[n/2+k-1]}, \; k = 1, \dots, n/2,$$

and defining the so-called *quasiderivatives* $\psi^{[k]}$,

$$\psi^{[k]} = \check{K}_x^{[k]} \psi, \tag{4.9}$$

by the recursion

$$\psi^{[k]} = \psi^{(k)}, \; k = 1, \dots, n/2 - 1, \; \psi^{[n/2]} = p_0 \psi^{(n/2)},$$
$$\psi^{[n/2+k]} = p_k \psi^{(n/2-k)} - d_x \psi^{[n/2+k-1]}, \; k = 1, \dots, n/2,$$

[4] This identification implies that we use a system of units where $\hbar = 1$.

we recall that $p_{n/2-k} = \phi_{2k}$; see (4.5). The recursive equations can be resolved to yield the following explicit representation for quasiderivatives[5]:

$$\psi^{[k]} = \psi^{(k)}, \; k = 0, \ldots, n/2 - 1,$$

$$\psi^{[n/2+k]} = \sum_{l=n/2-k}^{n/2} (-d_x)^{l+k-n/2}(\phi_{2l}\psi^{(l)}), \; k = 0, \ldots, n/2. \tag{4.10}$$

In these terms, the even s.a. differential operation (4.5) can be simply represented as

$$\check{f} = \check{K}_x^{[n]} \Longrightarrow \check{f}\psi = \psi^{[n]}. \tag{4.11}$$

For the representation (4.9)–(4.11) of even s.a. differential operations, the regularity conditions for the coefficient functions p_k can be considerably weakened: it is sufficient that the functions $p_1, \ldots, p_{n/2}, 1/p_0$ be locally integrable. An even s.a. differential operation of order n is then applicable to functions ψ that are a.c. in the interval (a, b) together with their quasiderivatives $\psi^{[k]}$, $k = 1, \ldots, n-1$. The definitions of regular and singular endpoints are modified accordingly.

In the theory of differential equations generated by even s.a. differential operations $\check{f}$, it is useful to introduce the *quasi-Wronskian* $\mathbb{W}\mathrm{r}\,(u_1, \ldots, u_n)$ of a set of functions u_i, $i = 1, \ldots, n$, instead of the ordinary Wronskian $\mathrm{Wr}\,(u_1, \ldots, u_n)$. We recall both definitions:

$$\mathbb{W}\mathrm{r}\,(u_1, \ldots, u_n) = \det \left|\mathbb{W}_{ij}\right|, \; \mathbb{W}_{ij} = u_j^{[i-1]},$$

$$\mathrm{Wr}\,(u_1, \ldots, u_n) = \det \left|\mathrm{W}_{ij}\right|, \; \mathrm{W}_{ij} = u_j^{(i-1)}, \; i, j = 1, \ldots, n;$$

see, e.g., [9, 116].

Both the quasi-Wronskian and the ordinary Wronskian are equal to zero for linearly dependent solutions u_i, $i = 1, \ldots, n$, of the equation $\check{f}u = 0$, but in contrast to the ordinary Wronskian, the quasi-Wronskian is a nonzero constant for a set of n linearly independent solutions.

As an example, we consider an s.a. differential operation of second order,

$$\check{f} = -d_x\,[p_0(x)d_x] + p_1(x).$$

In this case,

$$\check{K}_x^{[0]} = 1, \; \check{K}_x^{[1]} = p_0(x)d_x, \; \check{K}_x^{[2]} = p_1(x) - d_x\check{K}_x^{[1]} = \check{f},$$

$$\mathbb{W}\mathrm{r}\,(u_1, u_2) = u_1u_2^{[1]} - u_1^{[1]}u_2 = p_0(x)\mathrm{Wr}\,(u_1, u_2)\,.$$

---

[5]Quasiderivatives naturally emerge in this form when a product $\overline{\chi}\check{f}\psi$ is integrated by parts. The representation (4.10) can be taken as an independent definition of quasiderivatives. A similar representation evidently holds for quasiderivative differential operations.

For any s.a. differential operation $\check{f}$ of order n, the so-called *differential Lagrange identity*

$$\overline{\chi}\check{f}\psi - \left(\overline{\check{f}\chi}\right)\psi = d_x\left[\chi,\psi\right]_f \tag{4.12}$$

holds, where *the local sesquilinear form* $[\chi,\psi]_f(x)$ is a sesquilinear form in functions and their derivatives at the point x up to order $n-1$ (for $n=0$, this form is evidently zero).

The form $[\chi,\psi]_f$ is specific for each $\check{f}$; its coefficients are determined by the coefficients of $\check{f}$, but to simplify notation, we usually omit the generic subscript f if we speak about properties of the form that are common to all $\check{f}$ under consideration or if an origin of the form is clear from the context. For the general (mixed) s.a. differential operation $\check{f}$ (4.4), the local sesquilinear form $[\chi,\psi]_f$ is a sum of the corresponding partial forms for even s.a. monomials $\check{f}_{(2k)}$ and odd s.a. binomials $\check{f}_{(2k+1)}$ that constitute the $\check{f}$:

$$\begin{aligned}
[\chi,\psi]_f &= \sum_{l=1}^{n}[\chi,\psi]_{f_{(l)}},\\
[\chi,\psi]_{f_{(2k)}} &= -\sum_{l=0}^{k-1}\left[\overline{\chi}^{(l)}\left(-d_x\right)^{k-l-1}\left(\phi_{2k}\psi^{(k)}\right)-\left(\overline{\chi}\leftrightarrows\psi\right)\right],\ k\geq 1,\\
[\chi,\psi]_{f_{(2k+1)}} &= -i\,\overline{\chi}^{(k)}\phi_{2k+1}\psi^{(k)}+\frac{i}{2}\sum_{l=0}^{k-1}\Big\{\overline{\chi}^{(l)}(-d_x)^{k-l-1}\\
&\quad\times\left[\phi_{2k+1}\psi^{(k+1)}+\left(\phi_{2k+1}\psi^{(k)}\right)'\right]+\left(\overline{\chi}\leftrightarrows\psi\right)\Big\},\ k\geq 0.
\end{aligned}\tag{4.13}$$

For even s.a. differential operations of (even) order n, the local sesquilinear form $[\chi,\psi]_f$ is a simple sesquilinear form in quasiderivatives with coefficients ± 1:

$$[\chi,\psi]_f(x) = \sum_{k=0}^{n/2-1}\left(\overline{\chi^{[n-k-1]}}\psi^{[k]}-\overline{\chi^{[k]}}\psi^{[n-k-1]}\right). \tag{4.14}$$

As simple examples, we have $[\chi,\psi]_p(x) = -i\,\overline{\chi(x)}\psi(x)$, and

$$[\chi,\psi]_{\mathcal{H}}(x) = [\chi,\psi]_H(x) = \overline{\chi'(x)}\psi(x) - \overline{\chi(x)}\psi'(x), \tag{4.15}$$

for the respective first-order differential operation (4.6) and second-order differential operations (4.7) and (4.8). The simplest way of verifying the differential Lagrange identity (4.12) is by directly differentiating representations (4.13) and (4.14).

We now indicate some properties of the forms (4.13) and (4.14). We first warn the reader against possible confusion with notation: the symbol of the form, especially without a generic subscript, [,], coincides with the conventional symbol of a commutator. But the form does not possess the properties of a commutator, in particular, $[\psi,\psi] \neq 0$. The form is evidently anti-Hermitian, $\overline{[\chi,\psi]} = -[\psi,\chi]$. Therefore, its reduction to the diagonal $\chi = \psi$ defines the quadratic form $[\psi,\psi]$, which is pure imaginary, $\overline{[\psi,\psi]} = -[\psi,\psi]$. In addition, for even s.a. differential operations whose coefficients are real, we have $\overline{[\chi,\psi]} = \left[\overline{\chi},\overline{\psi}\right]$, whence it follows that $\left[\overline{\psi},\psi\right] \equiv 0$, while for odd s.a. differential operations whose coefficients are pure imaginary, we have $\overline{[\chi,\psi]} = -\left[\overline{\chi},\overline{\psi}\right]$.

It directly follows from (4.12) that the reduction of the local form $[\chi,\psi]_f$ to the space of solutions of the homogeneous equation $\check{f}u = 0$ is independent of x: $[\chi,\psi]_f = \text{const}$, if $\check{f}\psi = \check{f}\chi = 0$. We note that for even and odd s.a. differential operations with the respective real and pure imaginary coefficients, the corresponding complex-conjugate functions also satisfy the homogeneous equation. For even second-order s.a. differential operations, the form $[\chi,\psi]$ coincides with the quasi-Wronskian of the functions $\overline{\chi}$ and ψ up to a sign:

$$\mathbb{W}\mathrm{r}(\bar{\chi},\psi) = \overline{\chi(x)}\psi^{[1]}(x) - \overline{\chi^{[1]}(x)}\psi(x) = -[\chi,\psi]\,.$$

Similar assertions, obviously modified, hold for solutions of the eigenvalue problem $\check{f}u_\lambda = \lambda u_\lambda$, $\operatorname{Im}\lambda = 0$.

The differential Lagrange identity yields the *integral Lagrange identity*

$$\int_\alpha^\beta \mathrm{d}x\overline{\chi}\check{f}\psi - \int_\alpha^\beta \mathrm{d}x\overline{\check{f}\chi}\psi = [\chi,\psi]_f\,(x)\Big|_\alpha^\beta, \tag{4.16}$$

where $[\alpha,\beta] \subset (a,b)$.

If the corresponding integrals converge on the whole interval (a,b), so that we can set $\alpha = a$ and $\beta = b$ in the left-hand side of (4.16), the integral Lagrange identity is generalized to the whole interval in the form

$$\int_a^b \mathrm{d}x\overline{\chi}\check{f}\psi - \int_a^b \mathrm{d}x\overline{\check{f}\chi}\psi = [\chi,\psi]_f\,(x)\Big|_a^b = \lim_{\alpha\to a,\beta\to b}[\chi,\psi]_f\,(x)\Big|_\alpha^\beta. \tag{4.17}$$

The integrals certainly exist if one of the functions is compactly supported, for example, $\psi = \varphi \in \mathcal{D}(a,b)$. In this case, we evidently have $[\chi,\varphi]_f(x)\big|_a^b = 0$, and the integral Lagrange identity becomes an equality:

$$\int_a^b \mathrm{d}x\overline{\chi}\check{f}\varphi = \int_a^b \mathrm{d}x\overline{\check{f}\chi}\varphi,\ \forall\varphi \in \mathcal{D}(a,b), \tag{4.18}$$

which is an extension of equality (4.3).

The integral Lagrange identity makes it possible to evaluate the scalar-product-like integrals $\left(u_\mu, u_\lambda\right) = \int_a^b \mathrm{d}x\overline{u_\mu}u_\lambda$ for solutions of the eigenvalue problem, $\check{f}\, u_\lambda = \lambda u_\lambda$, $\check{f}\, u_\mu = \lambda u_\mu$, in terms of limit values of the corresponding local sesquilinear form[6]:

$$\int_a^b \mathrm{d}x\overline{u_\mu}u_\lambda = \frac{1}{\lambda - \overline{\mu}}\,[u_\mu, u_\lambda]\big|_a^b\,. \tag{4.19}$$

The functions u_λ and/or u_μ may not belong to the Hilbert space $L^2(a,b)$. In this case, by the integral $\int_a^b \mathrm{d}x\overline{u_\mu}u_\lambda$, we mean the limit $\lim\limits_{\alpha\to a,\beta\to b}\int_\alpha^\beta \mathrm{d}x\overline{u_\mu}u_\lambda$ in the sense of distributions. The representation (4.19) can be used, and is indeed used in the physics literature, for establishing the orthonormality relations between (generalized) eigenfunctions of physical observables.

4.2 Some Notions on Solutions of Ordinary Differential Equations

The theory of s.a. differential operators in $L^2\,(a,b)$ is based on the theory of ordinary differential equations, both homogeneous and inhomogeneous, on the interval (a,b). We therefore remind the reader of some necessary facts from this theory as applied to differential equations generated by s.a. differential operations on the interval (a,b) with special emphasis on their general solutions, including the so-called generalized solutions. As noted above, we restrict ourselves to the case in which possible nonintegrable singularities of the coefficient functions of the corresponding differential operations can be located only at the ends of the interval (a,b). For simplicity's sake, we also assume that these functions are smooth in the interval, but the conclusions obtained within this framework are appropriately extended to more general cases, about which we shall make some special remarks.

To make the exposition more illuminating for physicists, we present the basic points of the theory of ordinary differential equations by considering examples of differential equations generated by the s.a. first-order differential operation (4.6) and the second-order differential operation (4.8), widely encountered in physical applications. The extension to the general case is not a particular problem, and remarks in that direction are made where appropriate.

Regarding the s.a. differential operation (4.6), the general solutions of the corresponding homogeneous and inhomogeneous equations are obvious and well known. This allows a complete solution of the problem of constructing an s.a. differential operator (the momentum operator) associated with this differential operation on different intervals; see Chap. 6.

[6]In the physics literature, such integrals are called overlap integrals. The formula (4.19) that follows implies that the overlap integrals for solutions of the eigenvalue problem are determined by the asymptotic behavior of the eigenfunctions at the endpoints of the interval.

We therefore turn to differential operation (4.8), which defines an ordinary differential operator in a complex linear space of functions that are a.c. in the interval (a, b), together with their first derivatives, the square-integrability of the functions involved is not assumed in advance. By our facilitating convention, the potential V is assumed to be a smooth function in the interval, which does not exclude singular behavior of the potential at the ends of the interval. We note that from the standpoint of constructing associated s.a. operators, this condition is actually not too restrictive. For instance, let the potential $V(x)$ be not smooth, but locally bounded with possible steplike jumps. Any such potential can be approximated by a smooth potential V_{reg} such that the difference $\delta V(x) = V(x) - V_{\text{reg}}(x)$ is bounded. Then the operators $\hat{H}$ and $\hat{H}_{\text{reg}}$ associated with the respective differential operations (4.8) differ from each other by the bounded s.a. multiplication operator $\widehat{\delta V} = \delta V(x)$, defined everywhere, $\hat{H} = \hat{H}_{\text{reg}} + \widehat{\delta V}$, and therefore, they are s.a. or non-s.a. simultaneously; in other words, any s.a. operator $\hat{H}_{\text{reg}}$ is assigned the s.a. operator $\hat{H} = \hat{H}_{\text{reg}} + \widehat{\delta V}$ with the same domain, and vice versa.

In the above-mentioned space of functions, we first examine the homogeneous differential equation

$$\check{H}u = -u'' + V(x)u = 0 \tag{4.20}$$

and then the inhomogeneous differential equation

$$\check{H}y = -y'' + V(x)y = h(x), \tag{4.21}$$

where $h(x)$ is a locally integrable function.

It is known from the theory of ordinary differential equations that if $V(x)$ is locally integrable, then (4.20) has two linearly independent solutions u_1 and u_2, $\check{H}u_{1,2} = 0$, that form a fundamental system, in the sense that the general solution of (4.20) is given by

$$u(x) = c_1u_1(x) + c_2u_2(x), \tag{4.22}$$

where c_1 and c_2 are arbitrary complex constants; these constants are fixed by initial conditions for u and u' at some interior point of the interval (a, b) or at its regular endpoint. The linear independence of u_1 and u_2 is equivalent to the requirement[7] $\text{Wr}(u_1, u_2) \neq 0$.

It is evident that the fundamental system $u_{1,2}$ is defined up to a nonsingular linear transformation. For real-valued potentials, $V = \overline{V}$, the functions $u_{1,2}$ can also be chosen as real-valued. If the left endpoint a of the interval (a, b) is regular, in particular, V is integrable up to a, $\int_a^\beta \mathrm{d}x\,|V| < \infty$, $\beta < b$, then any solution (4.22) and its first derivative have finite limits at this endpoint; see Lemma 4.5 below. The same is true for the regular right endpoint b. In the case of singular endpoints, the

[7] In the case under consideration, the usual Wronskian coincides with the quasi-Wronskian.

fundamental solutions and/or their first derivatives can have no limits, in particular, can be infinite, at such endpoints. If the potential V is smooth in the interval (a, b), then any solution (4.22) is also smooth in this interval.

The general solution of the inhomogeneous equation (4.21) is given by

$$\begin{aligned} y(x) &= c_1 u_1(x) + c_2 u_2(x) \\ &\quad + \frac{1}{\mathrm{Wr}(u_1, u_2)} \left[u_1(x) \int_\alpha^x \mathrm{d}x' u_2 h + u_2(x) \int_x^\beta \mathrm{d}x' u_1 h \right], \end{aligned} \tag{4.23}$$

where α and β are some interior points of the interval (a, b), and c_1 and c_2 are arbitrary constants fixed by initial conditions for y and y' at some inner point of the interval (a, b) or at its regular endpoint. If the left endpoint a of the interval is regular, we can always take $\alpha = a$. This is also possible in case the endpoint a is singular if the corresponding integral is certainly convergent, for example, if the functions u_2 and h are square-integrable on the interval (a, x); the same is true for the right endpoint b.

We now examine the question of so-called generalized solutions of the homogeneous equation (4.20), i.e., the question of functions u satisfying the linear functional equation[8]

$$\left(u, \check{H}\phi\right) = \int_a^b \mathrm{d}x \overline{u} \check{H}\phi = 0, \ \forall \phi \in \mathcal{D}(a, b). \tag{4.24}$$

It is evident that any ordinary solution u of the homogeneous equation (4.20) is a generalized solution by virtue of the equality

$$\int_a^b \mathrm{d}x \overline{u} \check{H}\phi = \int_a^b \mathrm{d}x \overline{\check{H}u}\phi, \ \forall \phi \mathcal{D}(a, b), \tag{4.25}$$

which is a particular case of the integral Lagrange identity (4.18) with $\check{f} = \check{H}$ and $\chi = u$. We show that conversely, any generalized solution of the homogeneous equation under consideration is an ordinary solution, i.e., any solution of (4.24) is given by (4.22). We actually need a generalization of du Bois–Reymond lemma, Lemma 2.12. We obtain this generalization on the basis of two auxiliary lemmas, and it then becomes clear how the obtained result can be extended to differential equations of any order.

Lemma 4.1. *A function $\chi \in \mathcal{D}(a, b)$ can be represented as*

$$\chi = \check{H}\phi, \ \phi \in \mathcal{D}(a, b)$$

[8] For a smooth V, the function u in (4.24) can be considered a distribution; then the sign of the integral in (4.24) is symbolic; however, for our purposes it is sufficient to consider u a usual function.

iff χ is orthogonal to all solutions u of the homogeneous equation[9] *(4.20),*

$$(u,\chi)=\int_a^b \mathrm{d}x\overline{u(x)}\chi(x)=0,\ \forall u:\ \check{H}u=0, \tag{4.26}$$

which is equivalent to the orthogonality of the function χ to a fundamental system of solutions u_1 and u_2 of (4.20), $(u_1,\chi)=(u_2,\chi)=0$.

Proof. Necessity immediately follows from (4.25).

Sufficiency: Let the function $\chi\in\mathcal{D}(a,b)$ satisfy condition (4.26) and let $\mathrm{supp}\chi\subseteq[\gamma,\delta]\subset(a,b)$. We choose the particular solution ϕ of the inhomogeneous equation $\check{H}\phi=\chi$ given by (4.23) with $c_1=c_2=0, \alpha=a, \beta=b$,

$$\phi(x)=\frac{1}{\mathrm{Wr}(u_1,u_2)}\left[u_1(x)\int_a^x \mathrm{d}x'u_2\chi+u_2(x)\int_x^b \mathrm{d}x'u_1\chi\right];$$

we can set $\alpha=a$ and $\beta=b$ even if the interval (a,b) is infinite because of the compactness of the support of the function χ. Because the functions u_1,u_2, and χ are smooth, the function ϕ is also smooth; because of condition (4.26) and the compactness of the support of the function χ, we have $\phi=0$ for $x<\gamma$ and $x>\delta$, i.e., $\phi\in\mathcal{D}(a,b)$, which proves the lemma. □

Lemma 4.2. *Any function $\varphi\in\mathcal{D}(a,b)$ can be represented as follows:*

$$\varphi=c_1(\varphi)\varphi_1+c_2(\varphi)\varphi_2+\check{H}\phi,\ c_i(\varphi)=(u_i,\varphi),\ i=1,2,$$

where u_1 and u_2 form a fundamental system of solutions of (4.20) and φ_1, φ_2, and ϕ are functions from $D(a,b)$ such that

$$\left(u_i,\varphi_j\right)=\delta_{ij},\ i,j=1,2; \tag{4.27}$$

the functions φ_1 and φ_2 can be considered fixed functions, independent of φ.

Proof. We first prove the existence of a pair φ_1, φ_2 of functions with property (4.27). It is sufficient to demonstrate that there exists a pair ϕ_1, ϕ_2 of functions such that the matrix $A_{ij}=\left(u_i,\phi_j\right)$ is nonsingular, $\det A\neq 0$. Then the functions $\varphi_i=\left(A^{-1}\right)_{ji}\phi_j$ form the required pair. Let (α,β) be any finite interval inside the interval (a,b). The restrictions of the fundamental system u_1 and u_2 to this interval, i.e., u_1 and u_2, considered only for $x\in(\alpha,\beta)$, belong to $L^2(\alpha,\beta)$. The linear independence of u_1 and u_2 implies that the matrix $U_{ij}=\int_\alpha^\beta \mathrm{d}x\overline{u_i}u_j$ is nonsingular. Because $\mathcal{D}(\alpha,\beta)$ is dense in $L^2(\alpha,\beta)$, we can find some functions ϕ_1 and ϕ_2 from $\mathcal{D}(\alpha,\beta)$ arbitrarily close to the respective functions u_1 and u_2 on the interval (α,β).

[9] Although u is generally not square-integrable, the symbol (,) for the scalar product in (4.26) is correct because of the compactness of the support of the function χ.

It follows that the matrix $A_{ij} = \int_\alpha^\beta \mathrm{d}x \overline{u_i} \phi_j$ is also arbitrarily close to the matrix U, and therefore, the matrix A is also nonsingular. At this point, it remains to note that the function $\varphi - c_1(\varphi)\varphi_1 - c_2(\varphi)\varphi_2$ satisfies the condition of Lemma 4.1. □

We can now prove a lemma generalizing the du Bois–Reymond lemma, Lemma 2.12.

Lemma 4.3. *A locally integrable function u satisfies (4.24) iff u is smooth on* (a,b) *and satisfies the homogeneous equation (4.20). This implies that any generalized solution of the equation is a usual smooth solution.*

Proof. Sufficiency immediately follows from (4.25). Necessity is proved on the basis of Lemma 4.2. Let φ be an arbitrary function in $\mathcal{D}(a,b)$. By virtue of Lemma 4.2, we have the representation

$$\varphi - (u_1,\varphi)\varphi_1 - (u_2,\varphi)\varphi_2 = \check{H}\phi,$$

where φ_1, φ_2, and ϕ are some functions in $\mathcal{D}(a,b)$ and u_1, u_2 is a fundamental system of solutions of (4.20). Substituting the corresponding representation of $\check{H}\phi$ in the left-hand side of (4.24) and rearranging the obtained expression in an obvious way, we obtain that $(\forall\varphi \in \mathcal{D}(a,b))$

$$\begin{aligned}\left(u, \check{H}\phi\right) &= (u, \varphi - (u_1,\varphi)\varphi_1 - (u_2,\varphi)\varphi_2) \\ &= \left(u - \overline{(u,\varphi_1)}u_1 - \overline{(u,\varphi_2)}u_2, \varphi\right) \\ &= \int_\alpha^\beta \mathrm{d}x \overline{(u - c_1u_1 - c_2u_2)}\varphi = 0,\end{aligned}$$

where $c_i = (\varphi_i, u)$, $i = 1, 2$, are constants, whence it follows that $u = c_1u_1 + c_2u_2$; the representation (4.22) for u is a solution of (4.20). This completes the proof of the lemma. □

We note that the above-presented method of proving the lemma on the basis of the fundamental system of solutions of the homogeneous equation under consideration is obviously extended to the general case of homogeneous equations generated by differential operation (4.1) (not necessarily s.a.) with smooth coefficients.

Lemma 4.4. *A locally integrable function u satisfies the equation*

$$\left(u, \check{f}\phi\right) = \int_a^b \mathrm{d}x \overline{u} \check{f}\phi = 0, \ \forall\phi = \mathcal{D}(a,b)\,, \tag{4.28}$$

where $\check{f}$ *is an arbitrary nth-order differential operation (4.1) with smooth coefficient functions, iff u is smooth in* (a,b) *and satisfies the adjoint equation* $\check{f}^*u = 0$. *This implies that any generalized solution of (4.28) is an ordinary smooth solution of the adjoint equation. It is evident that if* $\check{f}$ *is an s.a. differential operation, then u satisfies the equation* $\check{f}u = 0$.

This statement is well known in the theory of distributions [88, 140].

An obviously modified similar statement can be extended to the general differential operation (4.1) with coefficients not necessarily smooth, but satisfying the standard conditions cited in Sect. 4.1. For even s.a. differential operations, a similar statement formulated in terms of quasiderivatives holds under the above-mentioned weakened conditions on the coefficient functions; see [9, 116].

This result provides a basis for evaluation of the adjoint of an initial symmetric operator associated with a given s.a. differential operation; see below.

As is known, an ordinary differential equation of order n can be reduced to a system of n first-order differential equations, so that any differential operation $\check{f}$ (4.1) is assigned a matrix differential operation of first order with $n \times n$ matrix coefficients, and vice versa. This reduction is useful for proving the solvability of homogeneous and inhomogeneous equations and for establishing the structure of their general solutions. In particular, it can be shown that under standard conditions on the coefficients, the solutions of both homogeneous, $\check{f}u = 0$, and inhomogeneous, $\check{f}y = h$, equations and their $n-1$ derivatives, all being a.c. in the interval, have finite boundary values at regular endpoints, or continuous up to such endpoints, and these boundary values can be arbitrary; for the inhomogeneous equation, it is required that its right-hand side h be locally integrable up to the regular (finite) endpoints. Needless to say, this is true for differential equations generated by s.a. differential operations. For differential equations generated by even s.a. differential operations, a similar assertion holds under weakened conditions on the coefficients with the replacement of derivatives by quasiderivatives.

After all this, the concluding remark of this section looks rather natural. The previous consideration and all that follows is directly generalized to matrix differential operations, i.e., to differential operations with matrix coefficients, generating systems of differential equations, both homogeneous and inhomogeneous, and their associated differential operators in Hilbert spaces of vector functions like $L^2(a,b) \oplus \cdots \oplus L^2(a,b)$, wherein vector functions are columns of square-integrable functions. Such matrix differential operators are inherent in both nonrelativistic and relativistic QM, describing in particular the radial motion of spinning particles, for example, the Dirac particles; see Chaps. 9 and 10.

4.3 Natural Domain

4.3.1 General Remarks

We are now in a position to proceed to constructing s.a. differential operators in $L^2(a,b)$ associated with s.a. differential operations (4.1) on the basis of the general theory of s.a. extensions of symmetric operators outlined in Chap. 3.

We begin with the so-called natural domain for the s.a. differential operation $\check{f}$ of order n defined on an interval (a,b).

Let $D^*_{\check{f}}(a,b)$ be a subspace of $L^2\,(a,b)$ of functions ψ_* a.c. in the interval (a,b) together with their derivatives of order up to $n-1$ and such that the functions $\check{f}\psi_*$ are square-integrable on the interval, i.e.,

$$D^*_{\check{f}}(a,b) = \left\{\psi_* : \psi_*, \psi'_*, \ldots, \psi_*^{(n-1)} \text{ a.c. in } (a,b);\ \psi_*,\ \check{f}\psi_* \in L^2(a,b)\right\}. \tag{4.29}$$

It is evident that $D^*_{\check{f}}(a,b)$ is the largest subspace of $L^2\,(a,b)$ on which a differential operator with the rule of action $\check{f}$ can be defined: the requirement of absolute continuity for functions $\psi_*, \psi'_*, \ldots, \psi_*^{(n-1)}$ in the interval (a,b) is necessary for the expression $\check{f}\psi_*$ to be meaningful, while the requirement that ψ_* and $\check{f}\psi_*$ belong to $L^2\,(a,b)$ is necessary for the expression $\check{f}\psi_*$ to define an operator in $L^2\,(a,b)$. We call the domain (4.29) *the natural domain* for an s.a. differential operation $\check{f}$ and let $\hat{f}^*$ denote the operator in $L^2\,(a,b)$ associated with this differential operation and defined on the natural domain, so that

$$\hat{f}^* : \begin{cases} D_{f^*} = D^*_{\check{f}}\,(a,b)\,, \\ \hat{f}^*\psi_* = \check{f}\psi_*,\ \ \forall\psi_* \in D^*_{\check{f}}\,(a,b)\,. \end{cases} \tag{4.30}$$

It is evident that the linear space $\mathcal{D}\,(a,b)$ of smooth functions with compact support belongs to the natural domain, $\mathcal{D}\,(a,b) \subset D^*_{\check{f}}\,(a,b)$, and because $\mathcal{D}\,(a,b)$ is dense in $L^2\,(a,b)$, the domain $D^*_{\check{f}}\,(a,b)$ is also dense in $L^2\,(a,b)$, so that the operator $\hat{f}^*$ is densely defined.

A function ψ_* belonging to the natural domain and its derivatives can be singular at an endpoint of the interval unless the endpoint is regular.

Lemma 4.5. *Let $D^*_{\check{f}}\,(a,b)$ be the natural domain for an s.a. differential operation $\check{f}$ of order n with regular endpoints, one or both. The functions belonging to $D^*_{\check{f}}\,(a,b)$ and their derivatives of order up to $n-1$ have finite boundary values at the regular endpoints, or are continuous up to these endpoints, and these boundary values can be arbitrary. For example, let a be a regular endpoint. Then*

$$\lim_{x\to a}\psi_*^{(k)}(x) = \psi_*^{(k)}(a) < \infty,\ \ k = 0,1,\ldots,n-1,\ \forall\psi_* \in D^*_{\check{f}}(a,b).$$

For even s.a. differential operations with appropriately modified natural domain (under weakened conditions on the coefficients), a similar assertion holds for quasiderivatives, for example,

$$\lim_{x\to a}\psi_*^{[k]}(x) = \psi_*^{[k]}(a) < \infty,\ \ k = 0,1,\ldots,n-1,\ \forall\psi_* \in D^*_{\check{f}}(a,b),$$

if the endpoint a is regular.

Proof. Any function $\psi_* \in D^*_{\check{f}}(a,b)$ can be considered a solution of the inhomogeneous differential equation

$$\check{f}\psi_*(x) = \eta(x), \tag{4.31}$$

where the right-hand side $\eta(x)$ is square-integrable on (a,b) and is therefore locally integrable up to the regular (finite) endpoints. It then remains to refer to the behavior of solutions of inhomogeneous differential equations at regular ends; see the penultimate paragraph of the previous section. □

As was mentioned above, in the physics literature and even in textbooks on QM for physicists, an s.a. differential operation $\check{f}$ is not infrequently identified with an observable, an s.a. operator $\hat{f}$ in $L^2(a,b)$, whereas the spectrum and eigenfunctions of this operator are searched for without any reservations about its domain. This actually implies that by the domain of $\hat{f}$ is implicitly meant the natural domain for $\check{f}$, i.e., by the observable is meant the operator $\hat{f}^*$, $\hat{f} = \hat{f}^*$: it is believed that the only requirements for an observable are the requirement of square-integrability for its eigenfunctions of bound states and the requirement of local square-integrability and "normalizability to δ-function" for its (generalized) eigenfunctions of continuous spectrum. This proves to be sufficient sometimes, but generally, this is not the case; see the paradoxes in Chap. 1 and the following chapters.

Therefore, the question we try to answer first is whether the operator $\hat{f}^*$ (4.30) associated with an s.a. operation $\check{f}$ and defined on the natural domain is really s.a. In general, to answer this question is not a simple task. A simpler preliminary task is to check the symmetricity of $\hat{f}^*$, which is a necessary condition for its self-adjointness. We note that in the physics literature, symmetricity is not infrequently identified with self-adjointness, which is wrong for unbounded operators. But for the operator $\hat{f}^*$, as we will see below, its symmetricity implies its self-adjointness because it is the adjoint of a symmetric operator. The general theory of s.a. extensions of symmetric operators, see Chap. 3, suggests that studies on possible symmetricity, and then self-adjointness, of the operator $\hat{f}^*$, or its restrictions, are conveniently carried out in terms of the asymmetry forms (3.9) and (3.10) for the operator $\hat{f}^*$. These forms are completely similar to the asymmetry forms for the adjoint of a symmetric operator[10] introduced in Sect. 3.2. The sesquilinear asymmetry form ω_{f^*} and the quadratic asymmetry form Δ_{f^*} are defined respectively by

$$\omega_{f^*}(\chi_*, \psi_*) = \int_a^b \mathrm{d}x \overline{\chi_*}\, \check{f}\psi_* - \int_a^b \mathrm{d}x\, \overline{\check{f}\chi_*}\psi_*,\ \forall \chi_*, \psi_* \in D^*_{\check{f}}(a,b), \tag{4.32}$$

[10] The more so, since $\hat{f}^*$ proves to be the adjoint of a symmetric operator; see below.

and

$$\Delta_{f^*}(\psi_*) = \int_a^b \mathrm{d}x \overline{\psi_*}\, \check{f} \psi_* - \int_a^b \mathrm{d}x\, \overline{\check{f}\psi_*}\, \psi_*,\ \forall \psi_* \in D^*_{\check{f}}(a,b), \tag{4.33}$$

where the form Δ_{f^*} is a reduction of the form ω_{f^*} to the diagonal $\chi_* = \psi_*$. The forms ω_{f^*} and Δ_{f^*} determine each other; the arguments are similar to those in Sect. 3.2; we use both for convenience. Each of these forms is a measure of asymmetricity of the operator $\hat{f}^*$: if the asymmetry forms are trivial, i.e., are identically zero, the operator $\hat{f}^*$ is symmetric, and vice versa. It is essential that the values of the asymmetry forms for the differential operator $\hat{f}^*$ are determined[11] by the asymptotic behavior of functions belonging to $D^*_{\check{f}}(a,b)$ at the endpoints a and b of the interval. Namely, the forms ω_{f^*} and Δ_{f^*} are expressed in terms of the boundary values of the respective local sesquilinear form $[\chi_*, \psi_*]_f$ (4.13), (4.14) and the local quadratic form $[\psi_*, \psi_*]_f$, the reduction of the local sesquilinear form to the diagonal $\chi_* = \psi_*$. Indeed, according to definition (4.32) and to the integral Lagrange identity (4.17), we have

$$\omega_{f^*}(\chi_*, \psi_*) = [\chi_*, \psi_*]_f(x)\big|_a^b,\ \forall \chi_*, \psi_* \in D^*_{\check{f}}(a,b), \tag{4.34}$$

where by definition,

$$[\chi_*, \psi_*]_f(a/b) = \lim_{x\to a/b} [\chi_*, \psi_*]_f(x). \tag{4.35}$$

Each of the boundary values (4.35) exists by itself because of the existence of the integrals on the right-hand side of (4.32). We note that their existence does not imply that the functions belonging to $D^*_{\check{f}}(a,b)$ and their (quasi)derivatives have finite boundary values at the endpoints of the interval, unless the endpoints are regular.

For the quadratic asymmetry form, we similarly have

$$\Delta_{f^*}(\psi_*) = [\psi_*, \psi_*]_f(x)\big|_a^b,\ \forall \psi_* \in D^*_{\check{f}}(a,b), \tag{4.36}$$

where

$$[\psi_*, \psi_*]_f(a/b) = \lim_{x\to a/b} [\psi_*, \psi_*]_f(x). \tag{4.37}$$

It is natural to call the boundary values (4.35) and (4.37) of the local forms the *boundary forms*, respectively the *sesquilinear boundary form* and *quadratic boundary form*. It is also natural to distinguish the left and right boundary forms defined on the respective left, a, and right, b, endpoints of the interval. It is significant that the left and right boundary forms are independent in the following

[11] As for any differential operator associated with an s.a. differential operation.

sense. Let us evaluate the left form $[\chi_*, \psi_*]_f\,(a)$ for some functions $\chi_*, \psi_* \in D^*_{\check{f}}(a,b)$. For any function χ_*, we can find a function $\widetilde{\chi}_* \in D^*_{\check{f}}$ coinciding with χ_* near the left endpoint a and vanishing near the right endpoint b, more exactly, $\widetilde{\chi}_* = \chi_*, a \le x < \alpha < b$ and $\widetilde{\chi}_* = 0, \alpha < \beta < x \le b$. For differential operations satisfying the standard conditions on the coefficients,[12] such a function can be obtained by multiplying χ_* by a steplike smooth function $\tilde{\theta}\,(x)$ equal to unity near $x = a$ and zero near $x = b$. Accordingly, we have $[\widetilde{\chi}_*, \psi_*]_f\,(a) = [\chi_*, \psi_*]_f\,(a)$, whereas $[\widetilde{\chi}_*, \psi_*]_f\,(b) = 0$. A similar argument holds for the right endpoint b. It follows that the condition for triviality of the asymmetry form ω_{f^*}, i.e., the condition for its identically vanishing $\omega_{f^*}\,(\chi_*, \psi_*) = 0$, $\forall \chi_*, \psi_* \in D^*_{\check{f}}(a,b)$, is equivalent to the condition for triviality of each of the left and right boundary forms (4.35) by itself, i.e., to the boundary conditions $[\chi_*, \psi_*]_f\,(a/b) = 0$, $\forall \psi_*, \chi_* \in D^*_{\check{f}}(a,b)$. This assertion is evidently extended to the boundary forms $[\psi_*, \psi_*]\,(a/b)$: the condition $\Delta_{f^*}\,(\psi_*) = 0$, $\forall \psi_* \in D^*_{\check{f}}(a,b)$ is equivalent to the boundary conditions $[\psi_*, \psi_*]_f\,(a/b) = 0$, $\forall \psi_* \in D^*_{\check{f}}(a,b)$.

We thus obtain that an answer to the question whether the operator $\hat{f}^*$ is symmetric (and consequently, s.a.), is determined by the respective triviality or nontriviality of the boundary forms, both left and right, i.e., by whether these forms vanish identically on $D^*_{\check{f}}(a,b)$. We briefly discuss a possible way to answer this question. For definiteness, we examine the boundary forms $[\psi_*, \psi_*]_f\,(a/b)$. As was mentioned above, the natural domain $D^*_{\check{f}}(a,b)$ can be defined as the subspace of square-integrable solutions ψ_* of the differential equations (4.31). Therefore, we can evaluate the boundary forms $[\psi_*, \psi_*]_f\,(a/b)$ by establishing the asymptotic behavior of the general solution ψ_* of (4.31) at the endpoints a and b of the interval under the subsidiary condition that ψ_* be square-integrable on (a,b), i.e., at the endpoints. If we can prove that the boundary forms $[\psi_*, \psi_*]_f\,(a/b)$ are trivial, we thus prove that the operator $\hat{f}^*$ is symmetric, and consequently s.a. What is more, we show below that in such a case, the operator $\hat{f}^*$ defined on the natural domain is a unique s.a. operator associated with an s.a. differential operation $\check{f}$. But if we can indicate at least one function $\psi_* \in D^*_{\check{f}}(a,b)$ such that, for instance, $[\psi_*, \psi_*](a) \neq 0$, we prove that the operator $\hat{f}^*$ is not symmetric and a fortiori is not s.a.

In the general case, the triviality or nontriviality of the boundary forms $[\psi_*, \psi_*]\,(a/b)$ depends on the type of the interval, whether it is infinite or finite, and on the behavior of the coefficients of $\check{f}$ at the endpoints of the interval, in particular, on whether the endpoints are regular or singular. We illustrate possible situations by the simple examples of s.a. second-order differential operations $\check{\mathcal{H}}$ (4.7) and $\check{H}$ (4.8).

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[12]For even differential expressions with the coefficients satisfying the weakened conditions, the existence of the functions $\widetilde{\chi}$ with the required properties can also be proved [9, 116].

We first examine the s.a. differential operation $\check{\mathcal{H}} = -\,d_x^2$ on the whole real axis $\mathbb{R}$. The natural domain $D^*_{\check{\mathcal{H}}}(\mathbb{R})$ for this operation is, see (4.29),

$$D^*_{\check{\mathcal{H}}}(\mathbb{R}) = \left\{\psi_* : \psi_*, \psi'_* \text{ a.c. in } \mathbb{R};\ \psi_*,\ \psi''_* \in L^2(\mathbb{R})\right\}.$$

By Lemma 2.14, the condition $\psi_* \in D^*_{\check{\mathcal{H}}}(\mathbb{R})$ implies that $\psi_*(x), \psi'_*(x) \overset{|x|\to\infty}{\longrightarrow} 0$, and consequently, the quadratic local form $[\psi_*, \psi_*]_{\mathcal{H}} = -(\overline{\psi_*}\psi'_* - \overline{\psi'_*}\psi_*)$, vanishes as $|x| \to \infty$. We thus obtain that the boundary forms $[\psi_*, \psi_*]_{\mathcal{H}}\,(\infty/-\infty)$ are trivial, which means that the operator $\widehat{\mathcal{H}}^*$ defined on the natural domain is symmetric and consequently is s.a., and is a unique s.a. operator associated with the s.a. differential operation $\check{\mathcal{H}}$ on the whole real axis. From the physical standpoint, this means that there is a unique s.a. Hamiltonian for a free nonrelativistic particle moving along the real axis.

4.3.2 Physical Examples

We now examine the s.a. differential operation

$$\check{H} = -d_x^2 + V(x), \quad V(x) \neq 0,$$

on the real axis. We first note that the formal expressions for the corresponding local forms for $\check{\mathcal{H}}$ and $\check{H}$ are the same, see (4.15), and therefore, the boundary forms for $\widehat{\mathcal{H}}^*$and $\hat{H}^*$ can differ only because of the difference of the respective natural domains, namely, the difference in the behavior of the functions belonging respectively to $D^*_{\check{\mathcal{H}}}(\mathbb{R})$ and $D^*_{\check{H}}(\mathbb{R})$ at the boundaries, here at $\pm\infty$.

If the potential $V(x)$ is a uniformly bounded function on the whole axis, the conditions $\psi''_* \in L^2(\mathbb{R})$ and $-\psi''_* + V\psi \in L^2(\mathbb{R})$ are equivalent, which implies that the natural domains for $\check{\mathcal{H}}$ and for $\check{H}$ are the same, $D^*_{\check{\mathcal{H}}}(\mathbb{R}) = D^*_{\check{H}}(\mathbb{R})$, and consequently, the boundary forms for $\widehat{\mathcal{H}}^*$ and for $\hat{H}^*$ are the same, i.e., the boundary forms for $\hat{H}^*$ are trivial as well as those for $\widehat{\mathcal{H}}^*$. This means that the operator $\hat{H}^*$ is a unique s.a. operator in $L^2(\mathbb{R})$ associated with the s.a. differential operation $\check{H}$ if the potential V is bounded.[13] From the physical standpoint, this means that there is a unique s.a. Hamiltonian for a nonrelativistic particle moving along the real axis in a bounded potential field.

If the potential $V(x)$ is only locally bounded, the self-adjointness or non-self-adjointness of the operator $\hat{H}^*$ is determined by the behavior of the potential at infinity. It seems useful to illustrate possible situations in advance. We show in

[13]Another way to make sure that this is correct is to note that $\hat{H}^* = \widehat{\mathcal{H}}^* + \hat{V}$, where $\hat{V} = V(x)$ is a bounded operator defined everywhere.

Chap. 7 that if the potential at infinity is bounded from below by a falling quadratic parabola, i.e., $V(x) > -Kx^2$, $K > 0$, as $x \to \pm\infty$, then the boundary forms for the operator $\hat{H}^*$ are trivial, which means that $\hat{H}^*$ is a unique s.a. operator associated with $\check{H}$. For example, $V(x) = kx^2/2$ evidently satisfies this criterion, and we conclude that the well-known textbook Hamiltonian $\hat{H}$ for a harmonic oscillator that is associated with the s.a. differential operation $\check{H} = -d_x^2 + kx^2/2$ is uniquely defined as the operator $\hat{H}^*$ with the natural domain $D^*_{\check{H}}(\mathbb{R})$. But if the potential falls at infinity more rapidly than $-Kx^2$ with an arbitrary $K > 0$ (of course, such a potential is rather exotic), the situation changes radically. For example, let $V(x) = -x^4$, so that we deal with the s.a. differential operation $\check{H} = -d_x^2 - x^4$. Let $\phi(x)$ be a smooth function exponentially decreasing as $x \to -\infty$ and such that $\phi = x^{-1}\exp\left(ix^3/3\right)$, $x > N > 0$. It is easy to verify that $\phi \in D^*_{\check{H}}(\mathbb{R})$ and $[\phi, \phi]_H(x) = -2i$ for $x > N$, but this means that the right boundary form $[\psi_*, \psi_*]_H(\infty)$ is nontrivial, and consequently, the operator $\hat{H}^*$ defined on the natural domain is not symmetric, a fortiori s.a., and cannot be considered a QM Hamiltonian for a particle moving along the real axis in the potential field $V(x) = -x^4$. A correct Hamiltonian in this case requires a refined definition; such a definition is possible, although it is not unique; see Sect. 7.3.

If at least one of the endpoints of the interval (a, b) is finite (a semiaxis or a finite interval), the self-adjointness of the operator $\hat{H}^*$ crucially depends on the behavior of the potential at finite endpoints. Let the left endpoint a be regular. Then by Lemma 4.5, the functions $\psi_* \in D^*_{\check{H}}(a, b)$ and their derivatives ψ'_* can take arbitrary values at this endpoint, which implies that the left boundary form $[\psi_*, \psi_*]_H(a)$ is nontrivial, and therefore, the operator $\hat{H}^*$ is not s.a. for any potential V, including $V = 0$. Again, a correct definition of an s.a. Hamiltonian in this case is possible, but is not unique, see Chaps. 7–9.

An important remark concerning QM is in order. In physics, differential operations[14] similar to (4.8) on the positive semiaxis are usually of three- or two-dimensional origin. Their standard sources are the problems of a QM description of a spatial motion of a particle in spherically symmetric or axially symmetric fields.

Let us consider a spinless particle in a spherically symmetric field $V(r)$, $r = |\mathbf{r}|$, where $\mathbf{r}$ is the three-dimensional position vector of the particle. Quantum states of such a particle are described by the wave functions $\psi(\mathbf{r}) \in L^2(\mathbb{R}^3)$, and its motion is governed by a Hamiltonian associated with the differential operation (in appropriate units) $\check{\mathbf{H}} = -\triangle + V(r)$, where $\triangle$ is the Laplacian. The problem of correctly describing the motion that incorporates correctly defining an s.a. Hamiltonian and finding its stationary states is usually solved by separating variables in the spherical coordinates r, θ, φ, i.e., by passing from the three-dimensional wave function $\psi(\mathbf{r})$ to the spherical partial waves: $\psi(\mathbf{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}(2l + 1)u_{lm}(r)Y_{lm}(\theta, \varphi)$, where Y_{lm} are spherical harmonics. The partial waves $u_{lm}(r)Y_{lm}(\theta, \varphi)$ describe the motion of the particle with certain values l and m of the respective angular

[14] "Hamiltonians" in the language of physics.

momentum and its z-projection. For each partial wave, the total Hamiltonian is reduced to the so-called radial Hamiltonian, which governs the radial motion of the particle.[15] The radial states are conveniently described in terms of the radial wave functions $\psi_{lm}(r) \in L^2(\mathbb{R}_+)$, which differ from the partial amplitudes $u_{lm}(r)$ by the factor r, $\psi_{lm}(r) = ru_{lm}(r)$. The radial Hamiltonians are then associated with the differential operations $\check{H}_l$ of the form (4.8), $\check{H}_l = -d_r^2 + V_l(r)$, where the partial potential $V_l(r)$ is given by $V_l(r) = V(r) + l(l+1)r^{-2}$ and contains the so-called centrifugal term $l(l+1)r^{-2}$ independent of m. If the initial three-dimensional potential $V(r)$ is nonsingular or has some admissible singularity at the origin (for a more exact definition of an admissible singularity, see [56]; in particular, the Coulomb singularity $1/r$ is admissible), the natural domain for the three-dimensional $\check{\mathbf{H}}$ consists of functions $\psi_*(\mathbf{r})$ sufficiently regular at the origin such that the partial amplitudes $u_{lm}(r)$ are finite at $r = 0$, and therefore, the radial wave functions $\psi_{lm}(r)$ must vanish at $r = 0$. This means that the natural domain $D^*_{\check{H}_l}(\mathbb{R}_+)$ for $\check{H}_l$ must be additionally restricted with the boundary condition $\psi_{lm}(0) = 0$. This boundary condition for the radial eigenfunctions is well known to physicists; in fact, it is essential only for s-waves, $l = 0$, because for $l \neq 0$, it holds automatically. By virtue of these conditions, the left boundary form is trivial on $D^*_{H_l}(\mathbb{R}_+)$. If the behavior of the potential at $+\infty$ is not exotic, for example, if $V(r) \to 0$ as $r \to \infty$, the right boundary form is also trivial. Therefore, the operator $\hat{H}_l$ associated with the differential operation $\check{H}_l$ and defined on the domain $D^*_{\check{H}_l}(\mathbb{R}_+)$ is s.a. and can be considered the radial Hamiltonian in accordance with textbooks.

This analysis is extended to the case in which the potential $V(r)$ is strongly singular and positive at the origin. But it fails if the potential is strongly singular and negative at the origin, for example, if $V = \alpha/r^2$, $\alpha < -1/4$ or $V = \alpha/r^\beta$, $\alpha < 0$, $\beta > 2$ as $r \to 0$; in such cases, the so-called "a fall to the center" occurs, see [5, 21, 118, 123, 151]. Again, s.a. Hamiltonians can be defined in these cases, but not uniquely.[16]

A completely similar analysis can be carried out for a particle in an axially symmetric field $V(\rho)$, where $\rho = |\mathbf{x}|$ and $\mathbf{x}$ is the two-dimensional position vector of the particle in the plane perpendicular to the symmetry axis. After separating the free motion along the symmetry axis, the problem is reduced to a description of a two-dimensional motion in the perpendicular plane. It is usually solved by separating the polar coordinates ρ, φ in the form $\psi(\mathbf{x}) = \sum_{m\in\mathbb{Z}} u_m(\rho)\exp(im\varphi)$, where the axial partial waves $u_m(\rho)\exp(im\varphi)$, $m \in \mathbb{Z}$, describe the states of the particle with certain values m of the angular-momentum projection. If we describe the radial states in terms of the wave functions $\psi_m(\rho) = \rho^{1/2}u_m(\rho) \in L^2(\mathbb{R}_+)$, which differ from the initial partial waves $u_m(\rho)$ by the factor $\rho^{1/2}$, then the radial Hamiltonians are

[15] We mean the reductions of the total Hamiltonian to the subspaces of partial waves with fixed l and m.

[16] Curiously, in these cases, we have $\psi_{lm}(r) \to 0$ as $r \to 0$, but $\psi'_{lm}(r) \to \infty$.

associated with the differential operations $\check{H}_m = -d_\rho^2 + V_m(\rho)$, where the partial potentials are given by $V_m(\rho) = V(\rho) + m^2\rho^{-2}$ and contain the centrifugal term $m^2\rho^{-2}$. It is evident that all we have said concerning the radial Hamiltonians of the spherically symmetric problem is extended to these radial Hamiltonians.

If both endpoints of the interval (a, b) are regular, the operator $\hat{H}^*$ associated with (4.8) is certainly not s.a. for any V, because both the left and the right boundary forms are nontrivial. Consequently, this operator cannot be considered a correctly defined s.a. QM Hamiltonian for a particle moving on a finite interval of the real axis, a Hamiltonian that provides a unitary evolution. In particular, this statement holds for the operator $\widehat{\mathcal{H}}^*$ associated with (4.7). That is, an s.a. Hamiltonian for a free particle on a finite interval cannot be defined on the natural domain.

Let us consider the one-dimensional Schrödinger equation on the interval (a, b) with a Hamiltonian $\hat{H}$. As a consequence of this equation, we have

$$\frac{\partial}{\partial t}\int_a^b |\psi|^2 \mathrm{d}x = -i\Delta_H(\psi) = -i[\psi, \psi]_H(x)|_a^b .$$

The physical interpretation is evident: the quadratic boundary form coincides, up to a constant factor, with the probability flux through the corresponding endpoint, and the nontriviality of the boundary forms implies that the particle can escape or enter the interval through its endpoints, which would imply the nonunitarity of evolution. Sometimes, a similar interpretation is possible in three-dimensional cases.

We usually ensure the self-adjointness of a QM Hamiltonian for a free particle on a finite interval with additional boundary conditions on the wave functions, conditions that provide the vanishing of the corresponding asymmetry form; such boundary conditions are called *s.a. boundary conditions*; see, e.g., [11]. The most familiar s.a. boundary conditions are the zero boundary conditions $\psi(a) = \psi(b) = 0$, which correspond to a particle in an "infinite potential well," and the periodic boundary conditions $\psi(a) = \psi(b)$, $\psi'(a) = \psi'(b)$, which correspond to "quantization in a box" customarily used in quantum-statistical physics.

4.3.3 Operators of Multiplication

4.3.3.1 Self-adjoint Operator of Multiplication by a Function

The simplest examples of s.a. operators that are s.a. when defined on natural domains are multiplication operators first mentioned in Sect. 2.3.4. Let all the coefficient functions in representation (4.1) for the general differential operation be zero except the lowest one, $f_k(x) = 0, k = 1, \ldots, n$, while $f_0(x) = V(x) \neq 0$, so that we deal with the operation $\check{f} \equiv \check{V}$, $\check{V}\psi(x) = V(x)\psi(x)$, of multiplication by a function; according to our terminology, see Sect. 4.1, this is a differential operation of order zero. For simplicity, we assume that $V(x)$ is a locally square-integrable function in the interval (a, b) (and as a consequence, is locally integrable). This requirement can be essentially weakened; see below. If $V(x) = x$ then $\check{V} = \check{x}$, $\check{x}\psi(x) = x\psi(x)$, is called the operation of multiplication by the independent variable x.

We consider the operator $\hat{V}$ associated with the operation $\check{V}$ and defined on its natural domain by[17]

$$\hat{V}: \begin{cases} D_V = D^*_{\check{V}}(a,b) = \left\{\psi : \psi(x), V(x)\psi(x) \in L^2(a,b)\right\}, \\ \hat{V}\psi(x) = V(x)\psi(x). \end{cases}$$

The following assertions hold.

Proposition 4.6. *If the function $V(x)$ is real, $V(x) = \overline{V(x)}$, then the operator $\hat{V}$ is s.a.*

Proof. First of all, it is evident that the operator $\hat{V}$ is densely defined, $\overline{D_V} = L^2(a,b)$, because $\mathcal{D}(a,b) \subset D_V$. It is easy to verify that $\hat{V}$ is a symmetric operator. Its adjoint $\hat{V}^+$ is also easily calculated. The corresponding defining equation (2.24) for the pairs of functions $\psi_* \in D_{V^+} \subset L^2(a,b)$ and $\eta = \hat{V}^+\psi_* \in L^2(a,b)$ is

$$\int_a^b dx\overline{\psi_*(x)}V(x)\psi(x) = \int_a^b dx\overline{\eta(x)}\psi(x), \ \forall\psi \in D_V. \tag{4.38}$$

We rewrite (4.38) as

$$\int_a^b dx\overline{[\eta(x) - V(x)\psi_*(x)]}\psi(x) = 0, \ \forall\psi \in D_V,$$

which is a linear equation for the function $\eta(x) - V(x)\psi_*(x)$. Because the functions η, V, and ψ_* are locally square-integrable, the function $\eta - V\psi_*$ is locally integrable as well as η and $V\psi_*$. It then follows from a generalization of Lemma 2.7 (see Remark 2.11) that $\eta(x) - V(x)\psi_*(x) = 0$ almost everywhere, or $\eta(x) = \hat{V}^+\psi_*(x) = V(x)\psi_*(x)$, which implies that $\hat{V}^+ \subseteq \hat{V}$. The inverse inclusion $\hat{V} \subseteq \hat{V}^+$ is evident, which means that $\hat{V}^+ = \hat{V}$. In conclusion, we note that the condition of local square-integrability can be weakened to the condition that $V(x)$ be finite almost everywhere and measurable [125, 130]. □

Proposition 4.7. *Let $|V(x)| \leq C$, $C > 0$, $\forall x \in (a,b)$. Then $\hat{V}$ is a bounded operator in $L^2(a,b)$ defined everywhere, and $\|\hat{V}\| \leq C$, which directly follows from the inequality*

$$\|\hat{V}\psi\|^2 = \int_a^b dx|V(x)|^2|\psi|^2 \leq C^2\int_a^b dx|\psi|^2 = C^2\|\psi\|^2, \ \forall\psi \in L^2(a,b).$$

[17] In fact, this is the operator $\hat{V}^*$ associated with the operation $\check{V} = V(x)$. For simplicity, we do not write here the superscript $*$.

As a consequence, if $V(x)$ is real and $|V(x)| \leq C$, then $\hat{V}$ is a bounded s.a. operator defined on all of $L^2(a,b)$.

4.3.3.2 Self-adjoint Operator of Multiplication by an Independent Variable

Let $V(x) = x$, i.e., we consider the operation $\check{V} = \check{x}$ of multiplication by an independent variable. The associated operator $\hat{x}$ defined on the natural domain $D_x = D^*_{\check{x}}(a,b) \in L^2(a,b)$ of $\check{x}$ is called the operator of multiplication by an independent variable.

I. Let $(a,b) = \mathbb{R}$. According to item (a) of Sect. 4.3.3.1, the operator $\hat{x}$ defined by

$$\hat{x} : \begin{cases} D_x = D^*_{\check{x}}(\mathbb{R}) = \left\{\psi : \psi, x\psi \in L^2(\mathbb{R})\right\}, \\ \hat{x}\psi(x) = x\psi(x), \end{cases}$$

is s.a.

The following assertions hold for this operator.

(a) The operator $\hat{x}$ is unbounded and cannot be defined on the whole Hilbert space, i.e., $D_x \neq L^2(\mathbb{R})$, although $\overline{D_x} = L^2(\mathbb{R})$.

Indeed, let $\{\psi_\alpha(x) \in L^2(\mathbb{R}),\ \alpha \in \mathbb{R}_+\}$ be a set of functions parameterized by a parameter $\alpha \in \mathbb{R}_+$, where

$$\psi_\alpha(x) = \begin{cases} \psi_{+\alpha}(x),\ x \geq 0, \\ 0,\ x < 0, \end{cases}, \quad \psi_{+\alpha}(x) = \frac{(1+x)^{-3/2-\alpha}}{\sqrt{2(1+\alpha)}},$$

$$\|\psi_\alpha\| = 1 \Longrightarrow \psi_\alpha \in L^2(\mathbb{R}),\ \forall\alpha \in \mathbb{R}_+.$$

For these functions, we have

$$\|\hat{x}\psi_\alpha\|^2 = \frac{1}{2(1+\alpha)}\int_0^\infty \frac{x^2 dx}{(1+x)^{3+2\alpha}} = \frac{1}{4\alpha(1+2\alpha)(1+\alpha)^2},$$

$$\|\hat{x}\psi_\alpha\| = \alpha^{-1/2}/2 + O(1) \text{ as } \alpha \to 0.$$

Because the norms of the vectors $\hat{x}\psi_\alpha$ become arbitrarily large as $\alpha \to 0$, the operator $\hat{x}$ is unbounded. Moreover, $\hat{x}$ is not defined on some vectors $\psi \in L^2(\mathbb{R})$, e.g., on the vector ψ_0, which proves that $D_x \neq L^2(\mathbb{R})$.

(b) The operator $\hat{x}$ has no eigenvalues and eigenfunctions, and spec $\hat{x} = \mathbb{R}$.

Indeed, the eigenvalue problem for the s.a. operator $\hat{x}$ is formulated as the equation

$$(\hat{x} - \lambda)\xi(x) = (x - \lambda)\xi(x) = 0 \tag{4.39}$$

for a number $\lambda \in \mathbb{R}$ and a function $\xi(x) \in L^2(\mathbb{R})$. By virtue of this equation, the function $\xi(x)$ differs from zero at only one point $x = \lambda$, which implies that this function belongs to the equivalence class of the zero function in $L^2(\mathbb{R})$; see Chap. 2. This means that (4.39) with any real λ has no nontrivial solutions in $L^2(\mathbb{R})$, i.e., no $\lambda \in \mathbb{R}$ can be an eigenvalue of $\hat{x}$.

It remains to prove that any $\lambda \in \mathbb{R}$ is a spectrum point of $\hat{x}$. Assume the contrary: let $\lambda_0 \in \mathbb{R}$, and let $\lambda_0 \notin \operatorname{spec} \hat{x}$. This means that λ_0 is a regular point of $\hat{x}$, and in particular, the equation

$$(\hat{x} - \lambda_0)\xi(x) = (x - \lambda_0)\xi(x) = \eta(x) \tag{4.40}$$

has a solution $\xi \in L^2(\mathbb{R})$ for any $\eta \in L^2(\mathbb{R})$. Let

$$\eta(x) = \begin{cases} 1, & |x - \lambda_0| \le 1, \\ 0, & |x - \lambda_0| > 1. \end{cases}$$

Because the homogeneous equation (4.39) has only trivial solutions, (4.40) has a unique solution,

$$\xi(x) = \begin{cases} (x - \lambda_0)^{-1}, & |x - \lambda_0| \le 1, \\ 0, & |x - \lambda_0| > 1, \end{cases}$$

which is not square-integrable on $\mathbb{R}$. This contradiction proves that $\operatorname{spec} \hat{x} = \mathbb{R}$.

II. Let $(a, b) = \mathbb{R}_+$. Similarly to the previous case, it is easy to prove that:

(a) The operator $\hat{x}$ defined on the natural domain $D^*_x(\mathbb{R}_+)$ is an s.a. unbounded operator.
(b) The operator $\hat{x}$ has no eigenvalues and eigenfunctions.
(c) $\operatorname{spec} \hat{x} = \mathbb{R}_+$.

Regarding item (c), we have only to verify that all $\lambda < 0$ are regular points of $\hat{x}$. Indeed, a unique solution of (4.40) with any $\lambda < 0$ is $\xi(x) = (x + |\lambda|)^{-1}\eta(x)$, so that $\xi(x) \in L^2(\mathbb{R}_+)$ for any $\eta(x) \in L^2(\mathbb{R}_+)$ and $\|\xi\| \le |\lambda|^{-1} \|\eta\|$.

III. Let (a, b) be a finite interval $[0, l]$. Similarly to the previous cases, it is easy to prove that:

(a) The operator $\hat{x}$ defined everywhere is a bounded s.a. operator in $L^2(0, l)$ and its norm is equal to l, $\|\hat{x}\| = l$ (in the case of an arbitrary finite interval $[a, b]$, we have $\|\hat{x}\| = \max(|a|, b)$).
(b) The operator $\hat{x}$ has no eigenvalues and eigenfunctions.
(c) $\operatorname{spec} \hat{x} = [0, l]$.

Regarding item (a), we have only to prove that $\|\hat{x}\| = l$. Because $|x| \le l$, we have $\|\hat{x}\| \le l$ according to item (b) in Sect. 4.3.3.1. Let $\{\xi_n(x)\}_1^\infty$ be a sequence of functions belonging to $L^2(0, l)$, where

$$\xi_n(x) = \begin{cases} 0, \ 0 \le x < l - n^{-1}, \\ n^{1/2}, \ l - n^{-1} \le x \le l, \end{cases} \qquad \|\xi_n\| = 1.$$

It is easy to verify that

$$\|\hat{x}\xi_n\|^2 = n \int_{l-n^{-1}}^{l} x^2 \mathrm{d}x > (l - n^{-1})^2,$$

so that we have the estimate $l - n^{-1} < \|\hat{x}\xi_n\| \le l$. Taking the limit $n \to \infty$, we obtain that $\|\hat{x}\| = l$.

4.4 Initial Symmetric Operator and Its Adjoint

Because the operator $\hat{f}^*$ associated with a given s.a. differential operation $\check{f}$ and defined on the natural domain $D^*_{\check{f}}(a,b)$ is generally not s.a., we turn to the canonical methods for constructing s.a. operators associated with $\check{f}$. To facilitate an exposition in some places, basic constructions are illustrated by the examples of differential operations with smooth coefficients. But all the main results are extended, with natural modifications, to the general case of nonsmooth coefficients under the above-mentioned conditions, which is indicated where appropriate or even formulated explicitly.

We start with the so-called *initial symmetric operator* $\hat{f}$ associated with $\check{f}$ and defined on a certain domain $D_f \subset D^*_{\check{f}}(a,b)$ that must be dense in $L^2(a,b)$ and ensure the symmetricity of $\hat{f}$. If the coefficient functions of $\check{f}$ are smooth in the interval (a,b), the subspace $\mathcal{D}(a,b)$ of compactly supported smooth functions is convenient (and natural) to take for D_f, so that the initial symmetric operator is defined by

$$\hat{f} : \begin{cases} D_f = \mathcal{D}(a,b), \\ \hat{f}\varphi = \check{f}\varphi, \ \forall\varphi \in \mathcal{D}(a,b). \end{cases} \tag{4.41}$$

The definition is correct because $\check{f}\varphi \in \mathcal{D}(a,b) \subset L^2(a,b)$ and both conditions for symmetricity of $\hat{f}$, see Sect. 2.7.1, are fulfilled: $\hat{f}$ is densely defined, $\overline{\mathcal{D}(a,b)} = L^2(a,b)$ by Theorem 2.6, and (2.29) coincides with (4.3), which manifests the self-adjointness of the differential operation $\check{f}$.

In some sense, the operator $\hat{f}$ is a minimum densely defined operator associated with $\check{f}$; other associated operators that follow are its extensions. In the case of the general s.a. differential operation (4.1), we can take the same $\hat{f}$ (4.41) for the initial symmetric operator; moreover, we believe that the domain of any operator associated with $\check{f}$ must contain the subspace of compactly supported smooth functions. We emphasize that the initial symmetric operator $\hat{f}$ is only symmetric, but not s.a., because its adjoint $\hat{f}^+$ is generally a nontrivial extension of $\hat{f}$; it is not even closed, $\hat{f} \subset \overline{\hat{f}}$, $\mathcal{D}(a,b) \subset D_{\overline{f}}$; see below.

The second step consists in evaluating the operator $\hat{f}^+$, the adjoint of the initial symmetric operator $\hat{f}$, by solving the defining equation (2.24), which in our case becomes[18]

$$\int_a^b \mathrm{d}x \overline{\psi_*} \check{f} \varphi = \int_a^b \mathrm{d}x \overline{\eta} \varphi, \ \forall \varphi \in D(a,b), \tag{4.42}$$

an equation for pairs of functions $\psi_* \in L^2(a,b)$ and $\eta = \hat{f}^+\psi_* \in L^2(a,b)$.

Theorem 4.8. *The operator $\hat{f}^+$ coincides with the operator $\hat{f}^*$ defined by (4.30), $\hat{f}^+ = \hat{f}^*$. In particular, its domain D_{f^+} is the natural domain $D^*_{\check{f}}(a,b)$. In other words, a pair of functions $\psi_* \in L^2(a,b)$ and $\eta \in L^2(a,b)$ is a solution of defining equation (4.42) iff $\psi_* \in D^*_{\check{f}}(a,b)$ and $\eta = \check{f}\psi_*$.*

Proof. Sufficiency is evident because of the integral Lagrange identity (4.18) with $\chi = \psi_*$. Necessity is proved as follows. Let a pair ψ_*, $\eta \in L^2(a,b)$ be a solution of (4.42), and let a function $\widetilde{\psi}_*$ be a certain solution of the inhomogeneous equation $\check{f}\widetilde{\psi}_* = \eta$. Such a function, a.c. in the interval (a,b) together with its $n-1$ derivatives, indeed exists, because the square-integrability of η implies its local integrability. We therefore can represent the right-hand side of defining equation (4.42) as

$$\int_a^b \mathrm{d}x\, \overline{\eta}\varphi = \int_a^b \mathrm{d}x\, \overline{\check{f}\widetilde{\psi}_*}\varphi = \int_a^b \mathrm{d}x \overline{\widetilde{\psi}_*}\, \check{f}\varphi,$$

using the same Lagrange identity, which reduces the defining equation to

$$\int_a^b \mathrm{d}x\, \overline{u}\check{f}\varphi = 0, \ u = \psi_* - \widetilde{\psi}_*, \forall \varphi \in \mathcal{D}(a,b),$$

the equation for the function u. By Lemma 4.4, the function u is an ordinary smooth solution of the homogeneous equation $\check{f}u = 0$. We thus obtain the representation $\psi_* = \widetilde{\psi}_* + u$ for the function ψ_*, where the properties of summands $\widetilde{\psi}_*$ and u allow the conclusion that ψ_* is a.c. in the interval (a,b) together with its $n-1$ derivatives and $\eta = \check{f}\psi_*$, which completes the proof of the theorem. □

As was mentioned above, this theorem is extended to the initial symmetric operator associated with the general s.a. differential operation (4.1) with coefficients satisfying the standard conditions.

For even s.a. differential operations, the conditions on the coefficients can be weakened to the conditions of absolute continuity for quasiderivatives; see [9, 116].

[18] It appears convenient to replace ξ_* in (2.24) by ψ_*, see immediately below, while ξ is naturally replaced with φ.

Now we present a generalization of Theorem 4.8 for the case of non-s.a. differential operations.

Theorem 4.9. *Let $\check{f}$ be a general differential operation (4.1), let $\hat{f}$ be the corresponding initial operator defined by (4.41), and let $\hat{f}^*$ be a differential operator associated with $\check{f}^*$ and defined on the natural domain $D^*_{\check{f}^*}(a,b)$ as $\hat{f}^*\psi_* = \check{f}^*\psi_*$, $\forall\psi_* \in D^*_{\check{f}^*}(a,b)$. Then the operator $\hat{f}^*$ coincides with the adjoint $\hat{f}^+$, i.e., $\hat{f}^* = \hat{f}^+$.*

The proof of Theorem 4.9 is completely similar to the proof of Theorem 4.8.

From this point on, we return to s.a. operations $\check{f}$. By virtue of Theorem 4.8, the asymmetry forms ω_{f+} and Δ_{f+} for the operator $\hat{f}^+$ coincide with the asymmetry forms ω_{f^*} (4.32) and Δ_{f^*} (4.33) introduced above and allow the respective representations (4.34) and (4.36) in terms of the respective boundary forms (4.35) and (4.37). According to the general theory of symmetric operators, see Sect. 3.2, if the adjoint operator $\hat{f}^+$ is symmetric, which is equivalent in our case to the triviality of the boundary forms (4.35) and (4.37), then this operator is automatically s.a., which implies that the initial symmetric operator $\hat{f}$ is essentially s.a., and its unique s.a. extension $\hat{f}_{\mathfrak{e}}$ is its closure coinciding with its adjoint, $\hat{f}_{\mathfrak{e}} = \overline{\hat{f}} = \hat{f}^+ = \hat{f}^*$. This justifies our preliminary assertions made in advance in the previous section and related to the operator $\hat{f}^*$ defined on the natural domain.

If the adjoint operator $\hat{f}^+$ is not symmetric, which is what occurs in the general case, in particular, in the case of regular endpoints, we must proceed to the next steps of the general program for constructing s.a. operators as s.a. extensions of the initial symmetric operator $\hat{f}$, or equivalently, s.a. restrictions of the adjoint operator[19] $\hat{f}^+$.

The next step is an evaluation of the deficient subspaces and the deficiency indices of the initial symmetric operator $\hat{f}$; see the beginning of Sect. 3.1 and Sect. 3.5.

An important remark is in order. In the mathematical literature, there is a tradition to choose $z = \mathrm{i}$ and $\bar{z} = -\mathrm{i}$ (we remind the reader that all $z \in \mathbb{C}_+$ or $z \in \mathbb{C}_-$ are equivalent) because all the variables are conventionally assumed to be dimensionless. But in physics, an initial symmetric operator $\hat{f}$ and its adjoint $\hat{f}^+$ are usually assigned a certain dimension,[20] the dimension of the generating differential operation $\check{f}$. It is therefore natural to choose $z = \kappa\mathrm{i}$ and $\bar{z} = -\kappa\mathrm{i}$, where κ is an arbitrary, but fixed, constant parameter of the corresponding dimension. It may happen that a differential operation $\check{f}$, as well as a parent classical theory, does not contain any scale parameter. However, in constructing a physical observable as

[19] In particular, the above-discussed additional boundary conditions on the wave functions belonging to the domain of the Hamiltonian $\hat{H}$, which are justified by physical arguments, actually define s.a. restrictions of the non-s.a. operator $\hat{H}^*$ defined on the natural domain.

[20] In conventional units, a certain degree of length or momentum (or energy).

an s.a. extension of an initial symmetric operator $\hat{f}$, the dimensional parameter κ can enter a quantum theory and acquire a physical meaning of a scale parameter, violating the scale invariance of the classical theory.

For convenience, we change notation[21] and let D_+ and D_- denote the respective deficient subspaces $\aleph_{-i\kappa}$ and $\aleph_{i\kappa}$ and accordingly let ψ_+ and ψ_- denote the functions belonging to the respective deficient subspaces D_+ and D_-, so that the deficient subspaces and the deficiency indices of an initial symmetric operator $\hat{f}$ are now defined by

$$D_\pm = \left\{\psi_\pm : \psi_\pm \in D^*_{\check{f}}(a,b)\,,\ \check{f}\psi_\pm = \pm i\kappa\psi_\pm\right\},\ m_\pm = \dim D_\pm. \tag{4.43}$$

In this notation, first von Neumann formulas (3.5) and (3.6) become

$$D_{f+} = D^*_{\check{f}}(a,b) = D_{\overline{f}} + D_+ + D_- \tag{4.44}$$

and

$$\psi_* = \underline{\psi} + \psi_+ + \psi_-,$$

while von Neumann formulas (3.18) and (3.19) for the respective sesquilinear asymmetry form ω_{f+} and quadratic asymmetry form Δ_{f+}, which are nontrivial only on the sum $D_+ + D_-$ of the deficient subspaces, become

$$\omega_{f+}(\chi_*, \psi_*) = 2i\kappa\left[(\chi_+, \psi_+) - (\chi_-, \psi_-)\right] \tag{4.45}$$

and

$$\Delta_{f+}(\psi_*) = 2i\kappa\left(\|\psi_+\|^2 - \|\psi_-\|^2\right).$$

Evaluating the deficient subspaces $D_\pm$ is equivalent to finding the systems $\{\psi_{\pm,k}\}_1^{m\pm}$ of all linearly independent square-integrable solutions of the respective homogeneous linear differential equations[22]

$$\left(\check{f} \mp i\kappa\right)\psi_\pm = 0. \tag{4.46}$$

We also need to fix somehow the orthonormalized basis functions $\{e_{\pm,k}\}_1^{m\pm}$ in $D_\pm$ by applying the standard procedure of orthogonalization to the systems[23] $\{\psi_{\pm,k}\}_1^{m\pm}$, so that for any $\psi_\pm \in D_\pm$, the representations

[21] We are following here a recent convention in the physics literature.

[22] In general, these sysyems are subsystems of the respective fundamental systems of solutions of (4.46), because the fundamental systems can contain non-square-integrable solutions.

[23] It is not obligatory to normalize the basis functions to unity; it is sufficient that their norms be the same.

$$\psi_{\pm} = \sum_{k=1}^{m_{\pm}} c_{\pm,k} e_{\pm,k}, \ \check{f} e_{\pm,k} = \pm \mathrm{i}\kappa e_{\pm,k}, \ (e_{\pm,k}, e_{\pm,l}) = \delta_{kl},$$
$$c_{\pm,k} = (e_{\pm,k}, \psi_{\pm}), \quad k, l = 1, \ldots, m_{\pm}, \tag{4.47}$$

hold.

This stage is the most laborious in the general case. It requires a certain experience in solving differential equations, including the theory of special functions; the particular features of a specific problem manifest themselves exactly at this stage. But there are several useful assertions relating to possible values of deficiency indices and requiring no specific calculations; we elaborate on them.

We first note that the deficiency indices $m_{\pm}$ of a symmetric differential operator $\hat{f}$ of order n associated with an s.a. differential operation $\check{f}$ of order n are always finite and do not exceed n. Indeed, the fundamental system of solutions of each of the homogeneous differential equations (4.46) contains exactly n functions; the additional requirement of their square-integrability may only decrease this number, so that in the general case, we have the restriction $0 \leq m_{\pm} \leq n$.

As follows from the equality $\hat{f}^{+} = \hat{f}^{*}$ and the discussion of the operator $\hat{f}^{*}$ carried out in the previous subsection, the deficiency indices of the initial symmetric operator $\hat{f}$ depend on the type of the endpoints of an interval under consideration, whether they are regular or singular. If an endpoint is regular, the general solution of each equation from the set (4.46) is square-integrable at this endpoint by Lemma 4.5; therefore, the square-integrability of the functions $\psi_{\pm}$ is determined by their square-integrability at singular endpoints.

Let an interval (a, b) be finite, and let $\check{f}$ be an arbitrary s.a. differential operation of order n on this interval. If $\check{f}$ is regular, i.e., both endpoints of the interval are regular, then $m_{\pm} = n$ for the associated initial symmetric operator $\hat{f}$. According to the main theorem, Theorem 3.4, there exists an n^2-parameter $U(n)$ family of s.a. operators associated with a given s.a. differential operation $\check{f}$ in this case. For example (see Chap. 6), the differential operation $\check{p}$ (4.6) on a finite interval generates a one-parameter $U(1)$ family of s.a. operators, each of which can be considered the QM momentum operator for a particle moving along a finite interval of the real axis. The differential operation $\check{\mathcal{H}}$ (4.7) generates a four-parameter $U(2)$ family of s.a. operators, each of which can be adopted as the QM energy operator for a free particle moving along a finite interval, and the same holds for the differential operation $\check{H}$ (4.8) if the potential $V(x)$ is integrable at both endpoints and therefore preserves the regularity of the endpoints. We thus obtain that for a particle moving along a finite interval of the real axis, the well-known s.a. differential operations (4.6)–(4.8) with a regular V do not define the corresponding QM observables in a unique way; each of the observables needs an additional specification. In what follows, we show that this specification is achieved by means of s.a. boundary conditions on the wave functions belonging to the domain of the observable, which was already mentioned at the end of the previous section. An optimistic remark in conclusion is that in the regular case, s.a. operators associated with any s.a. differential operation of any order do in fact exist.

If one or both endpoints of the interval are singular, the situation is not so optimistic in the general case. In particular, it is different for even s.a. differential operations with real coefficients, for odd differential operations with pure imaginary coefficients, and for mixed differential operations.

We dwell on initial differential symmetric operators associated with even s.a. differential operations; see [9, 116]. For brevity, we call them even symmetric operators. The deficiency indices of any even symmetric operator $\hat{f}$ are equal, $m_{\pm} = m$, irrespective of the type of the endpoints of the interval. Indeed, because the coefficients of $\check{f}$ are real, any square-integrable solution ψ_+ of the first of (4.46) is assigned a square-integrable solution $\psi_- = \overline{\psi_+}$ of the second equation, whereas the linear independence of solutions is preserved under complex conjugation. In particular, for basis functions $e_{\pm,k}$ in $D_{\pm}$, defined by (4.47), we can choose complex-conjugate functions such that $e_{-,k} = \overline{e_{+,k}}$, $k = 1, \dots, m$. Therefore, any even s.a. differential operation generates at least one s.a. operator in $L^2(a,b)$, in contrast to odd s.a. differential operations; see an example of a first-order differential operation $\check{p}$ in Chap. 6. In particular, for any interval (a,b), the Hamiltonian of a nonrelativistic particle associated with the differential operation $\check{H}$ (4.8) can be defined as an s.a. operator for any potential V, perhaps not uniquely.

Two other useful assertions about the deficiency indices of even symmetric operators are based on the notion of the dimension of a linear space modulo its subspace and on the boundary properties of the functions belonging to the domain of the closure of an even symmetric operator at regular endpoints. In addition, we need (3.5) from the first von Neumann theorem, Theorem 3.1, and item (ii) in Remark 3.3 concerning a relationship between the deficiency indices of a symmetric operator and its symmetric extension.

We first remind the reader of the notion of a linear factor space. Let L be a linear space, and let M be one of its subspaces, $M \subset L$. By definition, the factor space L/M (or the space L modulo the subspace M) is the linear space whose vectors are equivalence classes of vectors in L generated by the following equivalence relation: two vectors $\xi \in L$ and $\eta \in L$ are considered equivalent if their difference belongs to M, $\xi - \eta \in M$. The dimension of the factor space L/M is denoted by $\dim_M L$ and is called the dimension of L modulo M. Linearly independent vectors $\xi_1, \dots, \xi_k \in L$ are called linearly independent modulo M if no nontrivial linear combination $\sum_{i=1}^{k} c_i \xi_i$ belongs to M. If $\dim_M L = n$, then the maximum number of vectors belonging to L and linearly independent modulo M is equal to n, so that $k \le n$. Let L be a direct sum of two of its subspaces L_1 and L_2, $L = L_1 + L_2$. Then its dimension is the sum of the dimensions of these subspaces, $\dim L = \dim L_1 + \dim L_2$, whereas $\dim_{L_1} L = \dim L_2$ and $\dim_{L_2} L = \dim L_1$.

Information about the boundary properties of functions belonging to the domain of the closure of an even symmetric operator at a regular endpoint is preliminary; the closures of differential symmetric operators are discussed in detail in the next section. Let $\hat{f}$ be an even symmetric operator of order n and let $\overline{\hat{f}}$ be its closure with domain $D_{\overline{f}}$. It turns out that the functions belonging to $D_{\overline{f}}$ vanish at regular endpoints together with their $n-1$ quasiderivatives; for example, if the left endpoint a is regular, then $\underline{\psi} \in D_{\overline{f}}$ implies that $\underline{\psi}^{[k]}(a) = 0$, $k = 0, \ldots, n-1$.

After these short digressions, we return to the deficiency indices of even symmetric operators in the case that at least one of the endpoints of the interval is singular.

We have the following theorem:

Theorem 4.10. *Let $\hat{f}$ be the initial symmetric operator associated with an even s.a. differential operation $\check{f}$ of order n on an interval (a, b), and let one of the endpoints of the interval be regular, whereas the other will be assumed singular. Then the deficiency indices of $\hat{f}$, being equal, $m_{\pm} = m$, and bounded from above, $m \leq n$, are also bounded from below by $n/2$, so that the double-sided restriction*

$$n/2 \leq m \leq n \tag{4.48}$$

holds.

Proof. We must prove only the boundedness of m from below. Let $\overline{\hat{f}}$ with domain $D_{\overline{f}}$ be the closure of $\hat{f}$. By the first von Neumann formula (3.5), we have the representation $D^*_{\check{f}}(a, b) = D_{\overline{f}} + D_+ + D_-$ for the domain of the adjoint operator $\hat{f}^+$. It follows from this representation that

$$\dim_{D_{\overline{f}}} D^*_{\check{f}}(a, b) = \dim(D_+ + D_-) = \dim D_+ + \dim D_- = 2m,$$

which means that the maximum number of functions belonging to $D^*_{\check{f}}(a, b)$ and linearly independent modulo $D_{\overline{f}}$ is equal to $2m$. If we find a set $\{\psi_{*l}\}_1^n$ of functions belonging to $D^*_{\check{f}}(a, b)$ and linearly independent modulo $D_{\overline{f}}$, we prove that $2m \geq n$, which is required. By Lemma 4.5, the functions $\psi_* \in D^*_{\check{f}}(a, b)$ and their quasiderivatives $\psi_*^{[k]}$ of order up to $n-1$ are finite at a regular endpoint, let it be the endpoint a, and can take arbitrary values at this endpoint. This implies that there exists a set $\{\psi_{*l}\}_1^n$ of linearly independent functions in $D^*_{\check{f}}(a, b)$ such that the $n \times n$ matrix A, $A_l^k = \psi_{*l}^{[k]}(a)$, $l = 1, \ldots, n$, $k = 0, \ldots, n-1$, is nonsingular, $\det A \neq 0$. But these functions are also linearly independent modulo $D_{\overline{f}}$, i.e., the equality $\sum_l c_l \psi_{*l} = \underline{\psi} \in D_{\overline{f}}$ implies that $c_l = 0$, $\forall l$. Indeed, let $\sum_l c_l \psi_{*l} = \underline{\psi}$. By the above-cited assertion about the behavior of functions belonging to $D_{\overline{f}}$ at a regular endpoint, we know that $\underline{\psi}^{[k]}(a) = 0$, $k = 0, \ldots, n-1$, or $\sum_l c_l \psi_{*l}^{[k]}(a) = \sum_l A_l^k c_l = 0$, whence it follows that $c_l = 0$, $\forall l$, because the matrix A is nonsingular. This completes the proof of the theorem. $\square$

As an example, the deficiency indices of the initial symmetric operator $\hat{H}$ associated with the differential operation $\check{H}$ (4.8) on the semiaxis $\mathbb{R}_+$ with a potential V integrable at $x = 0$ can be $m = 1$ or $m = 2$, but not zero, depending on the behavior of the potential at infinity. This implies that the QM Hamiltonian for a particle on the semiaxis, even though the particle is free, cannot be defined uniquely as an s.a. operator in $L^2(\mathbb{R}_+)$ without some additional arguments. This fact has been known since the paper by Weyl [162], where the cases $m = 1$ and $m = 2$ were respectively called the cases of "limit point" and "limit circle," in accordance with the method of embedded circles used by Weyl.

If both ends of the interval (a, b) are singular, an evaluation of the deficiency indices of an initial symmetric operator $\hat{f}$ is reduced to the case of one regular endpoint and one singular endpoint by means of a special symmetric restriction of this operator and a comparison of the closures of this restriction and the initial operator.[24]

Let $\check{f}$ be an even s.a. differential operation of order n given on an interval (a, b), both ends of which are singular; let $\hat{f}$ be an initial symmetric operator; let $m_\pm = m$ be its deficiency indices, and let $\overline{\hat{f}}$ be its closure. Let c be an arbitrary, but fixed, interior point of the interval (a, b), $a < c < b$. We note that $L^2(a, b) = L^2(a, c) \oplus L^2(c, b)$. We examine the restrictions $\check{f}_-$ and $\check{f}_+$ of the initial s.a. differential operation $\check{f}$ to the respective intervals (a, c) and (c, b). It is evident that both differential operations are of the same order n, they are s.a., and the endpoint c, the right one for $\check{f}_-$ and the left one for $\check{f}_+$, is regular for each of them. Let $\hat{f}_-$ and $\hat{f}_+$ be respectively the initial symmetric operators in $L^2(a, c)$ and $L^2(c, b)$ associated with these differential operations, let $m_\pm^{(-)} = m^{(-)}$ and $m_\pm^{(+)} = m^{(+)}$ be their deficiency indices, and let $\overline{\hat{f}_-}$ and $\overline{\hat{f}_+}$ be their closures with the respective domains $D_{\overline{f_-}} \subset L^2(a, c)$ and $D_{\overline{f_+}} \subset L^2(c, b)$. Because the endpoint c is regular for both differential operations, the functions in both $D_{\overline{f_-}}$ and $D_{\overline{f_+}}$ vanish at the point c, together with their quasiderivatives of order up to $n - 1$.

We consider a new symmetric operator $\hat{f}_c$ in $L^2(a, b)$ associated with the same differential operation $\check{f}$; its domain D_{f_c} is a direct orthogonal sum of the subspaces $\mathcal{D}(a, c)$ and $\mathcal{D}(c, b)$, $D_{f_c} = \mathcal{D}(a, c) \oplus \mathcal{D}(c, b)$. It is evident that this operator is densely defined, $\overline{D_{f_c}} = L^2(a, b)$, and $D_{f_c} \subset \mathcal{D}(a, b) = D_f$, so that $\hat{f}_c$ is a symmetric operator, which is a specific symmetric restriction of the initial symmetric operator $\hat{f}$, $\hat{f}_c \subset \hat{f}$. Let $m_{c+} = m_{c-} = m_c$ be its deficiency indices, and let $\overline{\hat{f}_c}$ be its closure; it is evident that $\overline{\hat{f}_c} \subset \overline{\hat{f}}$.

It is of crucial importance to observe that the operator $\hat{f}_c$ is a direct sum of the operators $\hat{f}_-$ and $\hat{f}_+$, $\hat{f}_c = \hat{f}_- + \hat{f}_+$, whence it follows, first, that its deficiency indices are the sums of the corresponding deficiency indices of the summands, i.e.,

$$m_c = m^{(-)} + m^{(+)}, \tag{4.49}$$

[24]This is the starting point of the so-called method of splitting [116].

and second, that its closure $\overline{\hat{f}_c}$ is a direct sum of the closures $\overline{\hat{f}_-}$ and $\overline{\hat{f}_+}$ of the summands. But this means that the operator $\overline{\hat{f}_c}$ is a restriction of the operator $\overline{\hat{f}}$ to the domain $D_{\overline{f_c}} \subset D_{\overline{f}}$, which differs from $D_{\overline{f}}$ only by the subsidiary condition on the functions $\underline{\psi} \in D_{\overline{f}}$, namely, $\underline{\psi} \in D_{\overline{f_c}} \Rightarrow \underline{\psi} \in D_{\overline{f}}$, $\underline{\psi}^{[k]}(c) = 0$, $k = 0, 1, \ldots, n-1$, whence it follows that there exist exactly n, and not more, linearly independent functions belonging to $D_{\overline{f}}$ that do not satisfy this condition and are linearly independent modulo $D_{\overline{f_c}}$, i.e.,

$$\dim_{D_{\overline{f_c}}} D_{\overline{f}} = n. \tag{4.50}$$

Because the operator $\overline{\hat{f}}$ is a nontrivial symmetric extension of $\hat{f}_c$, the second von Neumann theorem, Theorem 3.2, is applicable to this operator. According to item (ii) in Remark 3.3, the dimension of $D_{\overline{f}}$ modulo $D_{\overline{f_c}}$ is equal to the difference of the deficiency indices of the operators[25] $\hat{f}$ and $\hat{f}_c$,

$$\dim_{D_{\overline{f_c}}} D_{\overline{f}} = m_c - m. \tag{4.51}$$

A comparison of (4.49)–(4.51) results in the relation

$$m = m^{(+)} + m^{(-)} - n \tag{4.52}$$

between the deficiency indices of the operator $\hat{f}$ and the deficiency indices of the operators $\hat{f}_\pm$. We note that this relation is consistent with the general restriction $0 \leq m \leq n$ for the deficiency indices of the operator $\hat{f}$ because by Theorem 4.10, we have $n/2 \leq m^{(\pm)} \leq n$ and therefore $n \leq m^{(+)} + m^{(-)} \leq 2n$. It is known that if both endpoints are singular, the deficiency indices can take any values between 0 and n [9, 116].

We note that in deducing relation (4.52), we actually don't use the fact that the endpoints a and b of the interval are singular, and consequently, relation (4.52) holds in the general case. If both endpoints are regular, then we have $m^{(\pm)} = n$ and relation (4.52) is reduced to the already known relation $m = n$. But if only one endpoint is regular, let it be a, we obtain a useful relation $m = m^{(+)}$, which, in particular, implies that the deficiency indices are independent of a choice of the position of the regular endpoint.

We now return to the main problem of constructing s.a. operators associated with a given s.a. differential operation $\check{f}$ on an interval (a, b) as s.a. extensions of the initial symmetric operator $\hat{f}$. Let the deficient subspaces $D_\pm$ and the deficiency indices $m_\pm$ of the symmetric operator $\hat{f}$ be considered to have been

---

[25]We recall that the deficiency indices of a symmetric operator and those of its closure are the same.

found. According to the main theorem, Theorem 3.4, there are three possibilities for s.a. extensions of this operator.

Let the deficiency indices be different, $m_+ \neq m_-$, which is possible only for odd or mixed s.a. differential operations $\check{f}$ with at least one singular endpoint. In this case, there are no s.a. extensions of the operator $\hat{f}$, i.e., there exist no s.a. differential operators associated with the given differential operation $\check{f}$.

Let both deficiency indices be equal to zero, $m_\pm = 0$; for even differential operations, this is possible only if both endpoints of the interval (a, b) are singular. In this case, the initial symmetric operator $\hat{f}$ is essentially s.a., and its unique s.a. extension is its closure $\overline{\hat{f}}$ identical with its adjoint, $\overline{\hat{f}} = \hat{f}^+ = \hat{f}^*$. In other words, there exists only one s.a. differential operator associated with the given differential operation $\check{f}$ and defined on the natural domain. As we mentioned in the previous section, this fact can be established without explicitly evaluating the deficient subspaces and deficiency indices of the operator $\hat{f}$ if we are able to prove that the asymmetry forms Δ_{f+} or ω_{f+} for the adjoint operator are trivial, i.e., identically equal to zero.

Let both deficiency indices be different from zero and equal, $m_\pm = m > 0$, which always holds if both endpoints of the interval are regular. In this case, there exists an m^2-parameter $U(m)$ family of s.a. extensions of the initial symmetric operator $\hat{f}$. In other words, there exists a nontrivial family $\{\hat{f}_U, U \in U(m)\}$ of s.a. operators associated with the given differential operation $\check{f}$, and the problem of their proper and convenient specification arises.

Of course, such a specification must follow Theorem 3.4.[26] But as we already mentioned in the introduction to this chapter, an application of the main theorem to differential operators has several distinctive features, the main peculiarity being that the asymmetry forms for adjoint operators are expressed in terms of boundary forms. We indicate two other features. First, any s.a. extension $\hat{f}_U$ of an initial symmetric operator $\hat{f}$ is simultaneously an s.a. extension of its closure $\overline{\hat{f}}$ with domain $D_{\overline{f}}$ and a symmetric restriction of its adjoint $\hat{f}^+$. All these operators are associated with the same initial differential operation $\check{f}$, which gives a common rule of action, but are defined on generally different domains $D_f \subset D_{\overline{f}} \subset D_{f_U} \subset D_{f+} = D^*_{\check{f}}(a, b)$ in $L^2(a, b)$. Therefore, a specification of an s.a. operator $\hat{f}_U$ associated with a given s.a. differential operation $\check{f}$ is completely determined by a specification of its domain D_{f_U}. The same concerns the closure $\overline{\hat{f}}$. Second, because the deficiency indices of an initial symmetric operator $\hat{f}$ are finite, $m < \infty$, the isometries $\hat{U} : D_+ \longmapsto D_-$ defining the s.a. extensions $\hat{f}_U$ are specified by $m \times m$ unitary matrices U.

[26] Of course taking into account the change of notation for some basic notions in this chapter in comparison with the previous one.

4.5 Self-adjoint Extensions in Terms of Closure and Deficient Subspaces

The main theorem, Theorem 3.4, furnishes two ways (or methods) for specifying s.a. operators associated with a given s.a. differential operation $\check{f}$ as s.a. extensions $\hat{f}_U$ of an initial symmetric operator $\hat{f}$. In this section, we dwell on the first way based on (3.34). This way requires the knowledge of both the deficient subspaces $D_\pm$ of the initial symmetric operator $\hat{f}$ and the domain $D_{\overline{f}}$ of its closure $\overline{\hat{f}}$. The domain $D_{\overline{f}}$ is given by (3.13), or equivalently by (3.16) or (3.17) in Chap. 3, which in our new notation adopted for differential operators reads

$$D_{\overline{f}} = \left\{ \underline{\psi} : \underline{\psi} \in D^*_{\check{f}}(a,b)\,;\; \omega_{f^+}(\psi_*, \underline{\psi}) = 0,\ \forall \psi_* \in D^*_{\check{f}}(a,b) \right\},$$

where the asymmetry form $\omega_{f^+}(\psi_*, \underline{\psi}) = \omega_{f^*}(\psi_*, \underline{\psi})$ is given by (4.34) in terms of boundary forms (4.35). Because of the independence of the left and right boundary forms, the condition $\omega_{f^+}(\psi_*, \underline{\psi}) = 0$, $\forall \psi_* \in D^*_{\check{f}}(a,b)$ reduces to a couple of independent implicit zero boundary conditions at the left and right endpoints of the interval (a,b), and we finally obtain that the domain $D_{\overline{f}}$ of the closure $\overline{\hat{f}}$ of the initial symmetric operator $\hat{f}$ associated with a given s.a. differential operation $\check{f}$ is given by

$$D_{\overline{f}} = \left\{ \underline{\psi} : \underline{\psi} \in D^*_{\check{f}}(a,b)\,;\; \left[\psi_*, \underline{\psi}\right]_f (a/b) = 0,\ \forall \psi_* \in D^*_{\check{f}}(a,b) \right\}. \tag{4.53}$$

In some cases, the implicit boundary conditions in (4.53) can be converted to explicit boundary conditions on functions $\underline{\psi} \in D_{\overline{f}}$ and their (quasi)derivatives. For example, let $\check{f}$ be an even s.a. differential operation of order n on the interval (a,b), and let the left endpoint a be regular. Then, the functions $\underline{\psi}$, as well as any functions $\psi_* \in D^*_{\check{f}}(a,b)$, take finite values at the endpoint a together with their $n-1$ quasiderivatives, and according to (4.14), the boundary condition $[\psi_*, \underline{\psi}]_f(a) = 0$, $\forall \psi_* \in D^*_{\check{f}}(a,b)$, becomes

$$\sum_{k=0}^{n/2-1} \left(\overline{\psi_*^{[k]}(a)}\underline{\psi}^{[n-k-1]}(a) - \overline{\psi_*^{[n-k-1]}(a)}\underline{\psi}^{[k]}(a) \right) = 0,\ \forall \psi_* \in D^*_{\check{f}}(a,b)\,.$$

Because the boundary values $\psi_*^{[k]}(a)$, $k = 0,\dots,n-1$, can be arbitrary, see Lemma 4.5, the implicit boundary condition $[\psi_*, \underline{\psi}](a) = 0$, $\forall \psi_* \in D^*_{\check{f}}(a,b)$, is equivalent to the explicit boundary conditions $\underline{\psi}^{[k]}(a) = 0$, $k = 0,\dots,n-1$. A similar assertion holds for the regular endpoint b. This result was announced in advance in the previous section. We thus obtain that the domain $D_{\overline{f}}$ of the closure

$\overline{\hat{f}}$ of the initial symmetric operator $\hat{f}$ associated with a regular even s.a. differential operation $\check{f}$ of order n is given by

$$D_{\overline{f}} = \left\{\underline{\psi} : \underline{\psi} \in D^*_{\check{f}}(a,b)\,;\ \underline{\psi}^{[k]}(a/b) = 0,\ k = 0,\ldots,n-1\right\}, \tag{4.54}$$

and if only one endpoint, let it be a, is regular, then $D_{\overline{f}}$ is given by

$$D_{\overline{f}} = \left\{\begin{array}{l} \underline{\psi} : \underline{\psi} \in D^*_{\check{f}}(a,b)\,;\ \psi^{[k]}(a) = 0,\ k = 0,\ldots,n-1, \\ \left[\psi_*, \underline{\psi}\right]_f(b) = 0,\ \forall \psi_* \in D^*_{\check{f}}(a,b) \end{array}\right\}. \tag{4.55}$$

Remark 4.11. These assertions are extended to the initial symmetric operator associated with any regular s.a. differential operation of order n with the replacement quasiderivatives by ordinary derivatives because, as is shown below, see Lemma 4.23, the corresponding boundary forms are finite nondegenerate forms in the boundary values of functions belonging to $D^*_{\check{f}}(a,b)$ and their $n-1$ derivatives.

As an illustration, we consider the simplest known second-order regular s.a. differential operation $\check{\mathcal{H}}$ (4.7) on an interval $[0,l]$. The domain $D_{\overline{\mathcal{H}}}$ of the closure $\overline{\widehat{\mathcal{H}}}$ of the initial symmetric operator $\widehat{\mathcal{H}}$ is given by

$$D_{\overline{\mathcal{H}}} = \left\{\underline{\psi} : \underline{\psi} \in D^*_{\check{\mathcal{H}}}(0,l)\,;\ \underline{\psi}(0) = \underline{\psi}(l) = \underline{\psi}'(0) = \underline{\psi}'(l) = 0\right\}. \tag{4.56}$$

We note that this domain is also the domain of the closure $\overline{\hat{H}}$ of the initial symmetric operator $\hat{H}$, associated with s.a. differential operation $\check{H}$ (4.8) if the potential V is bounded $|V(x)| < c < \infty$. If V is not bounded, but locally integrable, the domain $D_{\overline{H}}$ of the corresponding closure $\overline{\hat{H}}$ differs from (4.56) only by replacing the condition $\underline{\psi}'' \in L^2(0,l)$ with the condition $-\underline{\psi}'' + V\underline{\psi} \in L^2(0,l)$. We also note that both $\overline{\widehat{\mathcal{H}}}$ and $\overline{\hat{H}}$ are evidently symmetric, but not s.a. because of the additional zero boundary conditions on the derivatives.

Once the domain $D_{\overline{f}}$ has been established, we are able to formulate a theorem that describes all s.a. extensions of the initial symmetric operator $\hat{f}$. This theorem is actually a paraphrase of the main theorem in the part associated with (3.34).

Theorem 4.12. *If the initial symmetric operator $\hat{f}$ associated with an s.a. differential operation $\check{f}$ has nonzero deficiency indices $m_\pm = m > 0$, then all its s.a. extensions form an m^2-parameter $U(m)$ family $\left\{\hat{f}_U,\, U \in U(m)\right\}$. Each s.a. operator $\hat{f}_U$ is specified by a unitary $m \times m$ matrix $U = \left\|U_{jk}\right\|$ and is given by*

$$\hat{f}_U : \left\{\begin{array}{l} D_{f_U} = \left\{\begin{array}{l} \psi_U : \psi_U = \underline{\psi} + \sum_{k=1}^m c_k e_{U,k},\ e_{U,k} = e_{+,k} \\ + \sum_{j=1}^m U_{jk} e_{-,j},\ \forall \underline{\psi} \in D_{\overline{f}},\ \forall c_k,\ k = 1,\ldots,m \end{array}\right\}, \\ \hat{f}_U \psi_U = \check{f}\psi_U, \end{array}\right. \tag{4.57}$$

where $D_{\overline{f}}$ *is given by (4.53), or (4.54) or (4.55) if* $\check{f}$ *is even and respectively both or one of the endpoints of the interval is regular, while* $\{e_{\pm,k}\}_1^m$ *are some (arbitrary, but fixed) orthonormalized basis functions in the respective deficient subspaces* $D_\pm$ *given by (4.43) and (4.47). In the case of even* $\check{f}$*, we can take* $e_{-,k} = \overline{e_{+,k}}$.

As an illustration, we examine the same second-order regular differential operation $\check{\mathcal{H}}$ (4.7) on an interval $[0,l]$. Because $\check{\mathcal{H}}$ is even, of order 2, and regular, the deficiency indices $m_\pm$ of the initial symmetric operator $\widehat{\mathcal{H}}$ are equal and $m_\pm = m = 2$. It then follows from Theorem 4.12 that for the differential operation $\check{\mathcal{H}}$, we have a four-parameter family $\widehat{\mathcal{H}}_U$, $U \in U(2)$, of associated s.a. operators $\widehat{\mathcal{H}}_U$, which we describe in equivalent different ways below. According to our convention, we cite only the domain $D_{\mathcal{H}_U}$ of $\widehat{\mathcal{H}}_U$.

To simplify the description, it is convenient to choose the dimensional parameter κ in (4.43) as $2(\pi/l)^2$. For orthonormalized basis functions in the two-dimensional deficient subspaces $D_\pm$, it is natural to take the functions

$$
\begin{aligned}
&e_{+,1} = N \exp\rho,\ e_{+,2} = N \exp(\pi - \rho),\ \rho = (1-i)\,\pi x/l, \\
&e_{-,1} = \overline{e_{+,1}},\ e_{-,2} = \overline{e_{+,2}},\ N = \left(\mathrm{e}^{2\pi} - 1\right)^{-1/2} (2\pi/l)^{1/2}, \qquad (4.58)
\end{aligned}
$$

where N is a normalization factor. According to (4.57), the domain $D_{\mathcal{H}_U}$ of an s.a. operator $\widehat{\mathcal{H}}_U$ is given by

$$
D_{\mathcal{H}_U} = \left\{ \begin{array}{l} \psi_U : \psi_U = \underline{\psi} + \sum_{k=1}^2 c_k e_{U,k},\ e_{U,k} = e_{+k} \\ + \sum_{j=1}^2 U_{jk} \overline{e_{+,j}},\ \forall \underline{\psi} \in D_{\overline{f}},\ \forall c_k,\ k = 1,2 \end{array} \right\}, \qquad (4.59)
$$

where the domain $D_{\overline{\mathcal{H}}}$ is given by (4.56) and $U = U_{jk}$ is a unitary 2×2 matrix. The normalization factor N in (4.58) can be included in the coefficients c_1, c_2 and is irrelevant.

This specification of $D_{\mathcal{H}_U}$ in terms of $D_{\overline{\mathcal{H}}}$ and deficient subspaces $D_\pm$ seems to be inconvenient from the standpoint of a future spectral analysis of the s.a. operators $\widehat{\mathcal{H}}_U$ and is not adopted in physics, where we are used to dealing with s.a. boundary conditions on the wave functions ψ_U. These conditions equivalently specifying $D_{\mathcal{H}_U}$ are linear relations between the boundary values of the wave functions ψ_U and their first derivatives ψ_U', without mentioning the domain $D_{\overline{\mathcal{H}}}$.

When deducing s.a. boundary conditions in our case, we proceed from representation (4.59) for $\psi_U, \psi_U = \underline{\psi} + \sum_{k=1}^2 c_k e_{U,k}$, with a given U. Because functions $\underline{\psi}$ and $\underline{\psi}'$ vanish at the endpoints of the interval, the four boundary values of the functions ψ_U and ψ_U' are determined only by the second term $\sum_{k=1}^2 c_k e_{U,k}$, the deficient space contribution, namely, by the certain boundary values of the functions $e_{U,k}$ and $e_{U,k}'$, $k = 1, 2$, and by two arbitrary constants c_1 and c_2, which results in two relations between the boundary values of functions ψ_U and ψ_U' after excluding the constants $c_{1,2}$; these relations evidently depend on the unitary matrix U.

To obtain these relations, it is convenient to work in terms of two-component columns and 2×2 matrices. We introduce the two-component columns $\Psi_U(x) = \left(\psi_U(x)\diagup\psi'_U(x)\right)$ and $C = (c_1\diagup c_2)$, and 2×2 matrices

$$E_U(x) = \|E_{U,ak}(x)\|,\ E_{U,ak}(x) = e^{(a-1)}_{U,k}(x),\ a,k = 1,2.$$

It then follows from (4.59) that

$$\Psi_U(0) = E_U(0)C,\ \Psi_U(l) = E_U(l)C. \tag{4.60}$$

It turns out that the rank of the rectangular 4×2 matrix $(E_U(0)\diagup E_U(l))$ is maximal and is equal to 2. We could, therefore, express the constants c_1 and c_2 in terms of $\psi_U(0),\dots,\psi'_U(l)$ from one of the two relations in (4.60), then substitute the obtained expressions in the remaining two relations and thus obtain two linear relations between the boundary values of the functions belonging to $D_{\mathcal{H}_U}$ and their first derivatives. But it is more convenient to proceed as follows. We multiply the first and second relations in (4.60) from the left by the respective matrices $E^+_U(0)\mathcal{E}$ and $E^+_U(l)\mathcal{E}$, where $\mathcal{E} = -i\sigma^2$ and σ^2 is the Pauli matrix, which yields

$$E^+_U(0)\mathcal{E}\Psi_U(0) = E^+_U(0)\mathcal{E}E_U(0)C,\ \ E^+_U(l)\mathcal{E}\Psi_U(l) = E^+_U(l)\mathcal{E}E_U(l)C.$$

The crucial remark is that the matrix

$$R = \|R_{jk}\| = E^+_U(l)\mathcal{E}E_U(l) - E^+_U(0)\mathcal{E}E_U(0)$$

is zero. Indeed, using (4.15) written as

$$[\chi,\psi]_{\check{\mathcal{H}}}(x) = \sum_{a,b=1}^{2}\overline{\chi^{(a-1)}(x)}\mathcal{E}_{ab}\psi^{(b-1)}(x)$$

and representation (4.34) and (4.35) for ω_{f^*} with $\hat{f}^* = \widehat{\mathcal{H}}^* = \widehat{\mathcal{H}}^+$, it is easy to verify that the matrix elements of the matrix R are represented as $R_{jk} = [e_{U,j}, e_{U,k}](x)\big|_0^l = \omega_{\mathcal{H}^+}(e_{U,j}, e_{U,k})$ and are therefore equal to zero because the restriction of the asymmetry form $\omega_{\mathcal{H}^+}$ to $D_{\mathcal{H}_U}$, the domain of an s.a. operator, vanishes. This means that the relation

$$E^+_U(l)\mathcal{E}\Psi_U(l) = E^+_U(0)\mathcal{E}\Psi_U(0) \tag{4.61}$$

holds, which is equivalent to the relations

$$\left[e_{U,j},\psi_U\right]_{\check{\mathcal{H}}}(x)\big|_0^l = 0,\ j = 1,2. \tag{4.62}$$

Relations (4.61), or (4.62), are just the s.a. boundary conditions specifying an s.a. extension $\widehat{\mathcal{H}}_U$. We note that the explicit form of boundary conditions depends on a choice of the orthonormal basis functions $e_{\pm,j}$, $j = 1, 2$, in the deficient subspaces. But it is easy to trace that under a change of the orthogonal bases, s.a. boundary conditions specifying a given s.a. extension are replaced by equivalent s.a. boundary conditions related to the initial ones by a nonsingular linear transformation.

It is clear that the representation (4.59) for $\psi_U \in D_{\mathcal{H}_U}$ is restored from boundary conditions (4.61), or (4.62), by reversing the above consideration.

It is also clear how this consideration is extended to s.a. operators associated with regular even s.a. differential operations of any order.

4.6 Self-adjoint Extensions in Terms of Self-adjoint Boundary Conditions

In this section, we dwell on the second way provided by Theorem 3.4 for specifying s.a. operators associated with a given s.a. differential operation $\check{f}$ as s.a. extensions $\hat{f}_U$ of the initial symmetric operator $\hat{f}$.

This way is based on (3.35) and incorporates representation (4.34) and (4.35) of the asymmetry form ω_{f^+} for the adjoint $\hat{f}^+$ in terms of boundary forms, which allows specifying s.a. differential operators by s.a. boundary conditions. They are explicit or implicit depending on whether the endpoints of the interval are regular or singular; on singular endpoints, they are generally of implicit asymptotic character. There are different, but of course equivalent, versions of the formulation of s.a. boundary conditions.

We reformulate the corresponding part of the main theorem as applied to differential operators; the following theorem is an alternative to Theorem 4.12.

Theorem 4.13. *If the initial symmetric operator $\hat{f}$ associated with an s.a. differential operation $\check{f}$ on an interval (a, b) has nonzero deficiency indices $m_\pm = m > 0$, then all its s.a. extensions form an m^2-parameter family $\{\hat{f}_U, U \in U(m)\}$. Each s.a. operator $\hat{f}_U$ is specified by s.a. boundary conditions including a unitary $m \times m$ matrix $U = \|U_{lk}\|$ and is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{ \begin{array}{l} \psi_U : \psi_U \in D^*_{\check{f}}(a,b), \ [e_{U,k}, \psi_U]_f(x)|_a^b = 0, \\ e_{U,k} = e_{+,k} + \sum_{l=1}^m U_{lk} e_{-,l}, \ k = 1, \dots, m \end{array} \right\}, \\ \hat{f}_U \psi_U = \check{f} \psi_U, \end{cases} \tag{4.63}$$

where $\{e_{\pm,k}\}_1^m$ are some (arbitrary, but fixed) orthonormalized basis functions in the respective deficient subspaces $D_\pm$ of the operator $\hat{f}$ given by (4.43) and (4.47). In the case of even $\check{f}$, we can take $e_{-,k} = \overline{e_{+,k}}$.

Remark 4.14. (1) The equation (4.63) defines the s.a. operator $\hat{f}_U$ as a restriction of the adjoint operator $\hat{f}^+$ to the domain D_{f_U} specified by the s.a. boundary conditions that restrict the asymptotic behavior of functions $\psi_* \in D^*_{\check{f}}(a,b)$ at the endpoints of the interval. These boundary conditions considered as additional linear equations for the functions ψ_* are linearly independent. Indeed, let the relation

$$\sum_{k=1}^{m} \overline{c_k} \left[e_{U,k}, \psi_*\right]_f (x) \Big|_a^b = 0, \ \forall \psi_* \in D^*_{\check{f}}(a,b),$$

with some constants c_k hold. Because of the independence of the left and right sesquilinear boundary forms and because of their anti-Hermiticity, this relation is equivalent to the relations

$$\left[\psi_*, \sum_{k=1}^{m} c_k e_{U,k}\right]_f (a/b) = 0, \ \forall \psi_* \in D^*_{\check{f}}(a,b).$$

But by (4.53), this implies that $\sum_{k=1}^{m} c_k e_{U,k} \in D_{\overline{f}}$, which is possible only if all c_k, $k = 1, \ldots, m$, are zero, because the functions $\{e_{U,k}\}_1^m$ belonging to $D_+ + D_-$ are linearly independent modulo $D_{\overline{f}}$.

(2) We recall that the relations

$$\left[e_{U,k}, e_{U,l}\right](x)\big|_a^b = \omega_{f^+}(e_{U,k}, e_{U,l}) = 0, \ k,l = 1, \ldots, m, \tag{4.64}$$

hold, so that the functions $\{e_{U,k}\}_1^m$ belong to D_{f_U}, and any ψ_U allows the representation $\psi_U = \underline{\psi} + \sum_{k=1}^{m} c_k, e_{U,k}$, so that the operators $\hat{f}_U$ appearing in Theorems 4.12 and 4.13 are the same under the same matrix U and the same basis functions $\{e_{\pm,k}\}_1^m$ (see the proof of the main theorem).

The s.a. boundary conditions (4.63) in Theorem 4.13 are generally of implicit asymptotic character because the existence of the boundary forms does not imply the existence of boundary values of functions belonging to $D^*_{\check{f}}(a,b)$ and their (quasi)derivatives. But in some particular cases, these conditions become explicit boundary conditions for the functions and their (quasi)derivatives. We examine two cases of this kind.

The first one is the case of a regular even s.a. differential operation $\check{f}$ of (even) order n on a finite interval (a,b). We recall that in this case, representation (4.14) for the local form $[.,.]_f$ holds, the functions belonging to $D^*_{\check{f}}(a,b)$ and their $n-1$ quasiderivatives have finite boundary values at both endpoints of the interval, see Lemma 4.5, and the deficiency indices of the initial symmetric operator $\hat{f}$ are equal and maximum, $m_{\pm} = n$; see Sect. 4.4. Consequently, the s.a. boundary conditions can be written as

$$\sum_{l,m=1}^{n} \overline{e_{U,k}^{[l-1]}(x)} \mathcal{E}_{lm} \psi_U^{[m-1]}(x) \Big|_a^b = 0, \ k = 1, \ldots, n, \tag{4.65}$$

where the $n \times n$ matrix $\mathcal{E} = \|\mathcal{E}_{lm}\|$ is given by

$$\mathcal{E}_{lm} = \delta_{l,n+1-m} \epsilon \left(l - \frac{n+1}{2} \right), \ l, m = 1, \ldots, n, \tag{4.66}$$

and $\epsilon(-x) = -\epsilon(x)$, $\epsilon(x) = 1$ for $x > 0$.

The s.a. boundary conditions (4.65) are conveniently represented in a condensed form by introducing the two $n \times n$ matrices

$$E_U(a/b) = \|E_{U,lk}(a/b)\|, \ E_{U,lk}(a/b) = e_{U,k}^{[l-1]}(a/b), \tag{4.67}$$

and the two n-component columns $\Psi_U(a/b)$ with components $\Psi_{U\,k}(a/b)$,

$$\Psi_{Uk}(a/b) = \psi_U^{[k-1]}(a/b), \ k = 1, \ldots, n. \tag{4.68}$$

In this condensed notation, s.a. boundary conditions (4.65) become

$$E_U^+(b) \mathcal{E} \Psi_U(b) = E_U^+(a) \mathcal{E} \Psi_U(a). \tag{4.69}$$

We consider it useful to present a separate brief version of Theorem 4.13 for the case of regular differential operations using the condensed notation.

Theorem 4.15. *Let $\hat{f}$ be the initial symmetric operator associated with a regular even s.a. differential operation $\check{f}$ of order n on an interval (a, b). Then all its s.a. extensions $\hat{f}_U$ form an n^2-parameter $U(n)$ family $\{\hat{f}_U, U \in U(n)\}$; each s.a. operator $\hat{f}_U$ is specified by s.a. boundary conditions (4.69) including a unitary $n \times n$ matrix $U = \|U_{lk}\|$ and is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{ \begin{array}{l} \psi_U : \psi_U \in D^*_{\check{f}}(a, b), \\ E_U^+(b) \mathcal{E} \Psi_U(b) = E_U^+(a) \mathcal{E} \Psi_U(a) \end{array} \right\}, \\ \hat{f}_U \psi_U = \check{f} \psi_U, \end{cases}$$

where the matrices $\mathcal{E}$ and $E_U(a/b)$ and the columns $\Psi_U(a/b)$ are defined by the respective formulas (4.66), (4.67), and (4.68).

Remark 4.14 following Theorem 4.13 is modified for Theorem 4.15 as follows.

1. The s.a. boundary conditions (4.69) are linearly independent, which is equivalent to the assertion that the $2n \times n$ matrix $\mathbb{E}$ composed of the matrices $E_U(a)$ and $E_U(b)$ has maximal rank:

$$\mathbb{E} = \left(E_U(a) \diagup E_U(b)\right), \ \operatorname{rank}\mathbb{E} = n. \tag{4.70}$$

Indeed, similarly to the above proof of the linear independence of the boundary conditions we deduce that according to (4.54), the condition $\sum_{k=1}^{n} \mathbb{E}_{\alpha k} c_k = 0$ implies that $\sum_{k=1}^{m} c_k e_{U,k} \in D_{\bar{f}}$, which in turn implies that $c_k = 0$, $\forall k$.
2. Relations (4.64) are written as

$$E_U^+(b)\,\mathcal{E}E_U(b) = E_U^+(a)\,\mathcal{E}E_U(a)\,. \tag{4.71}$$

Of course, in practical applications, the condensed notation needs deciphering.

We also note that the matrices $E_U(a/b)$ with a given U depend on the choice of the dimensional parameter κ in (4.43), or in differential equations (4.46), defining the deficient subspaces $D_\pm$ and on the choice of the orthogonal basis $\{e_{\pm,k}\}_1^n$ in $D_\pm$. For example, if we change the orthogonal basis,

$$e_{+,k} \longmapsto \tilde{e}_{+,k} = \sum_{l=1}^{n} V_{+lk} e_{+,l}, \ e_{-,k} \longmapsto \tilde{e}_{-,k} = \sum_{l=1}^{n} V_{-lk} e_{-,l},$$

where the matrices $V_\pm$ are unitary, and the choice $V_- = \overline{V_+}$ is optional, then the matrix U for the same s.a. extension is changed for the matrix $\tilde{U} = V_-^{-1} U V_+$.

Theorem 4.15 is extended, appropriately modified, to s.a. operators associated with any regular s.a. differential operations $\check{f}$ with the replacement of quasiderivatives by ordinary derivatives. This remark is similar to Remark 4.11.

As an illustration, we consider the previous second-order regular differential operation $\check{\mathcal{H}}$ (4.7) on a finite interval $[0, l]$. It is easy to see that the s.a. boundary conditions specifying the associated s.a. differential operators $\widehat{\mathcal{H}}_U$ in accordance with Theorem 4.15 and given by (4.69), or (4.65), with $n = 2$ actually coincide with s.a. boundary conditions (4.61), or (4.62), obtained in the previous section as an illustration of Theorem 4.12. Such must be the case because the two ways for specifying s.a. differential operators presented by Theorems 4.12 and 4.15, the version of Theorem 4.13, are equivalent.

It seems interesting to present examples of s.a. operators corresponding to a particular choice of the unitary matrix U. Each $\widehat{\mathcal{H}}_U$ is a candidate for a Hamiltonian for a free particle on the interval $[0, l]$. It is sufficient to indicate the corresponding s.a. boundary conditions. Henceforth, when presenting explicit boundary conditions corresponding to a particular choice of the matrix U, we conventionally omit the subscript U in the notation of the functions belonging to $D_{\mathcal{H}_U}$.

Choosing $U = I$, where I is the 2×2 identity matrix, we obtain the Hamiltonian $\widehat{\mathcal{H}}_I$ specified by s.a. boundary conditions, which, written in the conventional expanded form, looks rather exotic:

$$\begin{aligned}\psi(l) &= -\cosh\pi\,\psi(0) - l\pi^{-1}\sinh\pi\,\psi'(0),\\ \psi'(l) &= -l\pi^{-1}\sinh\pi\,\psi(0) - \cosh\pi\,\psi'(0).\end{aligned} \tag{4.72}$$

Choosing $U = -I$, we obtain the Hamiltonian $\widehat{\mathcal{H}}_{-I}$ specified by the familiar s.a. boundary conditions

$$\psi(0) = \psi(l) = 0 \tag{4.73}$$

and describing the behavior of a particle in an infinite square potential well.

Choosing $U = iI$, we obtain the Hamiltonian $\widehat{\mathcal{H}}_{iI}$ specified by the s.a. boundary conditions

$$\psi'(0) = \psi'(l) = 0. \tag{4.74}$$

Choosing $U = -\left[(1-i)\,I + (1+i)\,\sigma^1\right]/2$, where σ^1 is the Pauli matrix, we obtain the Hamiltonian $\widehat{\mathcal{H}}_U$ specified by the periodic boundary conditions[27]

$$\psi(0) = \psi(l),\ \psi'(0) = \psi'(l), \tag{4.75}$$

which are conventionally adopted in quantizing an ideal gas in a box.

We now examine the second case, in which the s.a. boundary conditions in Theorem 4.13 can be made into a conventional explicit form in terms of the boundary values of functions and their (quasi) derivatives. It is rather evident after the above discussion that such a possibility is realized for a singular even s.a. differential operation with one regular endpoint and one singular endpoint if the boundary form at the singular endpoint is trivial, i.e., vanishes identically. We only need to clear up the deficiency indices of the initial symmetric operator associated with such an s.a. differential operation in order to know the number of basis functions $e_{U,k}$, and therefore, the number of boundary conditions. It turns out that these two questions are interrelated: the boundary form at the singular endpoint is trivial if the deficiency indices of the initial symmetric operator are a minimum of possible ones, i.e., if $m_\pm = n/2$; see Theorem 4.10. We formulate this assertion as a lemma.

Lemma 4.16. *Let the deficiency indices of the initial symmetric operator $\hat{f}$ associated with an even s.a. differential operation $\check{f}$ of order n on an interval (a,b) with one regular endpoint, let it be a, and one singular endpoint, b, be minimum, $m_\pm = n/2$. Then the boundary form at the singular endpoint is trivial,*

$$[\chi_*, \psi_*](b) = 0,\ \forall \chi_*, \psi_* \in D^*_{\check{f}}(a,b). \tag{4.76}$$

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[27] It must be confessed that in this case we actually solve the inverse problem of finding a matrix U that yields periodic boundary conditions.

If the endpoint a is singular, while the endpoint b is regular, then b in (4.76) must be replaced by a.

Proof. A proof of the lemma is based on the arguments used in proving the independence of the boundary forms at different endpoints, see Sect. 4.3, and on the arguments used in proving Theorem 4.10. Because the endpoint a is regular, there exist n functions $w_k \in D^*_{\check{f}}(a,b)$, $k = 1,\ldots,n$, vanishing near the singular endpoint b and linearly independent modulo $D_{\overline{f}}$. On the other hand, by the condition of the lemma, the deficiency indices of the operator $\hat{f}$, as well of $\hat{f}$, are equal to $n/2$, and therefore, the dimension of the subspace $D^*_{\check{f}}(a,b)$ modulo $D_{\overline{f}}$ is equal to $n/2 + n/2 = n$, $\dim_{D_{\overline{f}}} D^*_{\check{f}}(a,b) = n$. The latter means that any function $\psi_* \in D^*_{\check{f}}(a,b)$ can be represented as $\psi_* = \underline{\psi} + \sum_{k=1}^{n} c_k w_k$, where $\underline{\psi} \in D_{\overline{f}}$ and c_k are some coefficients. Consequently, the boundary form $[\chi_*, \psi_*](b)$ for any $\chi_*, \psi_* \in D^*_{\check{f}}(a,b)$ can be represented as

$$[\chi_*, \psi_*](b) = [\chi_*, \underline{\psi}](b) + \sum_{k=1}^{n} c_k [\chi_*, w_k](b).$$

The first term on the right-hand side of the last equality vanishes due to (4.53), while the second term vanishes because all functions w_k vanish near the singular endpoint b, which proves the lemma. □

In the next section, we show that conversely, if the boundary form at a singular endpoint is trivial, then the deficiency indices of the initial symmetric operator are minimum, $m_\pm = n/2$.

It follows from Lemma 4.16 that in the case under consideration, the terms $[e_{U,k}, \psi_U](b)$ in boundary conditions (4.63) in Theorem 4.13 vanish, and the boundary conditions reduce to

$$[e_{U,k}, \psi_U](a) = 0, \ k = 1,\ldots,n/2.$$

Using arguments similar to those in deducing (4.65), we represent these boundary conditions in an explicit form

$$\sum_{l,m=1}^{n} \overline{e_{U,k}^{[l-1]}(a)} \mathcal{E}_{lm} \psi_U^{[m-1]}(a) = 0, \ k = 1,\ldots,n/2, \tag{4.77}$$

where $\mathcal{E}_{lm}$ are given by (4.66). If we introduce a rectangular $n \times n/2$ matrix $E_{1/2,U}(a)$ with the matrix elements

$$\left(E_{1/2,U}(a)\right)_{lk} = e_{U,k}^{[l-1]}(a), \ l = 1,\ldots,n, \ k = 1,\ldots,n/2, \tag{4.78}$$

then s.a. boundary conditions (4.77) are represented in a condensed form as

$$E^{+}_{1/2,U}\,(a)\,\mathcal{E}\Psi\,(a) = 0, \tag{4.79}$$

where $\Psi\,(a)$ is given by (4.68).

We consider it useful to present a separate brief version of Theorem 4.13 for the case under consideration using the condensed notation.

Theorem 4.17. *Let $\check{f}$ be an even s.a. differential operation of order n on an interval (a,b) with a regular endpoint a and a singular endpoint b, and let the associated initial symmetric operator $\hat{f}$ have the minimum possible deficiency indices $m_{\pm} = n/2$, which is equivalent to the triviality of the boundary form at the singular endpoint b. Then all s.a. extensions $\hat{f}_U$ of $\hat{f}$ form an $(n/2)^2$-parameter family $\{\hat{f}_U, U \in U(n/2)\}$; each s.a. operator $\hat{f}_U$ is specified by s.a. boundary conditions (4.79) and is given by*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\psi_U : \psi_U \in D^*_{\check{f}}\,(a,b)\,,\; E^{+}_{1/2,U}\,(a)\,\mathcal{E}\Psi_U\,(a) = 0\right\}, \\ \hat{f}_U\psi_U = \check{f}\psi_U\,, \end{cases} \tag{4.80}$$

where the matrices $\mathcal{E}$ and $E_{1/2,U}\,(a)$ are defined respectively by (4.66) and (4.78) and the column $\Psi_U\,(a)$ is defined by (4.68). If the endpoint a is singular, while the endpoint b is regular, then a in (4.80) is replaced by b.

Remark 4.14 following Theorem 4.13 is modified for Theorem 4.17 as follows:

1. The s.a. boundary conditions (4.79) are linearly independent, or equivalently, the rectangular $n\times n/2$ matrix $E_{1/2,U}\,(a)$ has maximum rank, $\operatorname{rank}E_{1/2,U}\,(a) = n/2$, which is an analogue of (4.70).
2. Relation (4.64) becomes $E^{+}_{1/2,U}\,(a)\,\mathcal{E}E_{1/2,U}\,(a) = 0$, which is an analogue of relation (4.71).

In Sect. 6.2, we consider the s.a. operators associated with the s.a. differential operation $\check{\mathcal{H}}$ (4.7) on the semiaxis $\mathbb{R}_+$ as an illustration of Theorem 4.17.

Specifying the s.a. differential operators $\hat{f}_U$ by means of s.a. boundary conditions according to Theorems 4.13, 4.15, and 4.17 requires evaluating the orthonormal basis functions $\{e_{\pm,k}\}_1^m$ in the corresponding deficient subspaces $D_{\pm}$. But it is only the behavior of these functions at the boundary that is essential. In addition, there is an arbitrariness in the choice of these functions, while examples show (see Chaps. 6–9) that their specific boundary values actually do not enter into the answer. All this allows us to suggest that many analytic details are irrelevant from the standpoint of the general construction. Indeed, there exists another way of specifying s.a. boundary conditions that allows us to avoid a detailed evaluation of deficient subspaces, a way whereby the analytic problem is reduced significantly and is actually replaced by some algebraic problem. This way may turn out to be more convenient for applications. It is based on an equivalent, but modified, version of the main theorem in the part associated with (3.35).

We emphasize that all that follows up to Theorem 4.20 is concerned with general operators, not only differential ones.

We recall representation (3.35) for the domain D_{f_U} of an s.a. extension $\hat{f}_U$ with the deficiency indices $m_\pm = m$, $0 < m < \infty$. For future convenience, we take $z = i\kappa$ and use a naturally changed notation[28]:

$$\aleph_{\bar{z}} \to D_+,\ \xi_z \to \xi_+,\ e_{z,k} \to e_{+,k},\ \aleph_z \to D_-,\ \xi_{\bar{z}} \to \xi_-,\ e_{\bar{z},k} \to e_{-,k}.$$

Then the representation (3.35) becomes

$$D_{f_U} = \left\{ \begin{array}{l} \xi_U : \xi_U \in D_{f^+};\ \omega_{f^+}(e_{U,k}, \xi_U) = 0, \\ e_{U,k} = e_{+,k} + \sum_{l=1}^m U_{lk} e_{-,l},\ k = 1, \dots, m \end{array} \right\}, \tag{4.81}$$

where $\{e_{\pm,k}\}_1^m$ are the orthogonal bases in the respective deficient subspaces $D_\pm$ and $U = \|U_{lk}\|$ is a unitary $m \times m$ matrix.

The two properties are characteristic for the vectors $e_{U,k}$: first, the vectors $e_{U,k}$, $k = 1, \dots, m$, form a basis in the subspace $(\hat{I} + \hat{U})D_+$ and are linearly independent modulo $D_{\overline{f}}$, and second, because each of them belongs to D_{f_U}, the relations

$$\omega_{f^+}(e_{U,k}, e_{U,l}) = 0,\ k, l = 1, \dots, m, \tag{4.82}$$

hold.[29] It turns out that in fact, it is only the linear independence of these m vectors modulo $D_{\overline{f}}$ and relations (4.82) for them, and not their specific form, that are of importance.

Indeed, the vectors $e_{U,k}$ in representation (4.81) can be equivalently replaced by their nondegenerate linear combinations,

$$e_{U,k} \to w_{U,k} = \sum_{a=1}^m X_{ak} e_{U,a},$$

where the matrix $X = \|X_{ak}\|$ is nonsingular. Similar to $\{e_{U,k}\}_1^m$, the vectors $\{w_{U,k}\}_1^m$ form a basis in the subspace $(\hat{I} + \hat{U})D_+$ and are linearly independent modulo $D_{\overline{f}}$, and relations (4.82) are also evidently extended to these vectors, $\omega_{f^+}(w_{U,k}, w_{U,l}) = 0$. In addition, we can add an arbitrary vector $\underline{\xi}_k$ belonging to the domain $D_{\overline{f}}$ of the closure $\overline{f}$ to any vector $w_{U,k}$,

$$w_{U,k} \to w_k = w_{U,k} + \underline{\xi}_k = \sum_{a=1}^m X_{ak} e_{U,k} + \underline{\xi}_k,\ \underline{\xi}_k \in D_{\overline{f}}, \tag{4.83}$$

[28] Following the above convention for differential operators.

[29] These properties as applied to differential operators were already cited above.

and obtain an equivalent representation of the domain D_{f_U} in terms of the new m vectors $\{w_k\}_1^m$ (4.83):

$$D_{f_U} = \left\{\xi_U : \xi_U \in D_{f^+};\ \omega_{f^+}(w_k, \xi_U) = 0,\ \forall k\right\}, \tag{4.84}$$

because $\omega_{f^+}(\underline{\xi}_k, \xi_U) = \overline{\omega_{f^+}(\xi_U, \underline{\xi}_k)} = 0$ according to the defining property (3.17) of the domain $D_{\overline{f}}$. For the same reason, relations (4.82) hold for the new m vectors $\{w_k\}_1^m$,

$$\omega_{f^+}(w_k, w_l) = 0,\ k, l = 1, \dots, m. \tag{4.85}$$

It is also evident that these new vectors are linearly independent modulo $D_{\overline{f}}$.

It turns out that the inverse also holds. Namely, let $\hat{f}$ be a symmetric operator; let $\overline{\hat{f}}$ be its closure; let $\hat{f}^+$ be its adjoint, and let the deficiency indices of $\hat{f}$ be finite, equal, and different from zero, $m_\pm = m$, $0 < m < \infty$, so that $D_f \subseteq D_{\overline{f}} \subset D_{f^+}$ and $\dim_{D_{\overline{f}}} D_{f^+} = 2m$. Let $\{w_k\}_1^m$ be a set of vectors with the following properties:

(1) $w_k \in D_{f^+}$, $k = 1, \dots, m$.
(2) all w_k are linearly independent modulo $D_{\overline{f}}$, i.e.,

$$\sum_{k=1}^m c_k w_k \in D_{\overline{f}},\ \forall c_k \in \mathbb{C} \Longrightarrow c_k = 0,\ \forall k.$$

(3) The vectors w_k, $k = 1, \dots, m$, satisfy relations (4.85).

Then the set of vectors $\{w_k\}_1^m$ defines some s.a. extension $\hat{f}_U$ of the symmetric operator $\hat{f}$ as an s.a. restriction of its adjoint $\hat{f}^+$, $\hat{f} \subset \hat{f}_U = \hat{f}_U^+ \subset \hat{f}^+$, to the domain D_{f_U} belonging to D_{f^+} and given by (4.84).

To prove this assertion, it is sufficient to prove that all the vectors w_k can be represented as

$$w_k = \sum_{a=1}^m X_{ak}\left(e_{+,a} + \sum_{b=1}^m U_{ba} e_{-,b}\right) + \underline{\xi}_k,\ \forall k,$$

where $\{e_{\pm,k}\}_1^m$ are some orthogonal bases in the respective deficient subspaces $D_\pm$ of the initial symmetric operator $\hat{f}$, X_{ak} and U_{ba} are some coefficients such that the $m \times m$ matrix $X = \|X_{ak}\|$ is nonsingular, the $m \times m$ matrix $U = \|U_{ba}\|$ is unitary, and all the vectors $\underline{\xi}_k$ belong to $D_{\overline{f}}$.

We first turn to the condition (1). According to the first von Neumann formula (3.6), any vector w_k belonging to D_{f^+} is uniquely represented (taking the change of notation into account) as

$$w_k = \xi_{+,k} + \xi_{-,k} + \underline{\xi}_k = \sum_{a=1}^m X_{ak} e_{+,a} + \sum_{a=1}^m Y_{ak} e_{-,a} + \underline{\xi}_k,$$

where $\xi_{\pm,k} \in D_{\pm}$, $\underline{\xi}_k \in D_{\overline{f}}$, and X_{ak} and Y_{ak} are some coefficients. We then turn to the conditions (2) and (3). The crucial remark is that according to these conditions, both $m \times m$ matrices $X = \|X_{ak}\|$ and $Y = \|Y_{ak}\|$ are nonsingular. The proof is by contradiction. Let, for instance, the rank of the matrix X be not maximal, rank $X < m$, which means that there exists a set $\{c_k\}_1^m$ of complex numbers c_k such that at least one of them is different from zero, while $\sum_{k=1}^m X_{ak}c_k = 0$, $\forall a$. In such a case, we have

$$\sum_{k=1}^{m} c_k \xi_{+,k} = \sum_{a=1}^{m} \left(\sum_{k=1}^{m} X_{ak} c_k \right) e_{+,a} = 0,$$

and the vector $w = \sum_{k=1}^m c_k w_k$ is represented as

$$w = \xi_- + \underline{\xi},\ \xi_- = \sum_{k=1}^{m} c_k \xi_{-,k},\ \underline{\xi} = \sum_{k=1}^{m} c_k \underline{\xi}_k.$$

According to the condition (3), we have

$$\omega_{f+}(w, w) = \Delta_{f+}(w) = \sum_{k,l=1}^{m} \bar{c}_k c_l \omega_{f+}(w_k, w_l) = 0.$$

On the other hand, by the von Neumann formula (3.19) for the quadratic asymmetry form Δ_{f+}, we have that $\Delta_{f+}(w) = -2\mathrm{i}\kappa \|\xi_-\|^2$, whence it follows that $\xi_- = 0$, and therefore $w = \underline{\xi} \in D_{\bar{f}}$. Condition (2) then implies that all the numbers c_k are equal to zero, which is a contradiction that proves the nonsingularity of the matrix X.

The proof of the nonsingularity of the matrix Y is similar.

The nonsingularity of the matrix X allows representing the vectors w_k as follows:

$$w_k = \sum_{a=1}^{m} X_{ak} \left(e_{+,a} + \sum_{b=1}^{m} U_{ba} e_{-,b} \right) + \underline{\xi}_k,\ k = 1, \ldots, m,$$

where the nonsingular $m \times m$ matrix U is given by $U = YX^{-1}$. Using representation (3.18) for the asymmetry form ω_{f+}, condition (3) can be written as

$$\omega_{f+}(w_k, w_l) = 2\mathrm{i}\kappa \left[(\xi_{+,k}, \xi_{+,l}) - (\xi_{-,k}, \xi_{-,l}) \right] = 0,\ \forall k, l,$$

which is reduced to

$$\sum_{a,b=1}^{m} \left[\overline{X}_{ak} (e_{+,a}, e_{+,b}) X_{bl} - \overline{Y}_{ak} (e_{-,a}, e_{-,b}) Y_{bl} \right] = \sum_{a=1}^{m} \left[\overline{X}_{ak} X_{al} - \overline{Y}_{ak} Y_{al} \right] = 0$$

by virtue of the orthonormalization relations $(e_{\pm,a}, e_{\pm,b}) = \delta_{ab}$. The last equality can be represented in matrix form as

$$X^+X - Y^+Y = X^+\left[I - \left(\left(X^+\right)^{-1} Y^+\right)\left(YX^{-1}\right)\right]X = X^+\left(I - U^+U\right)X = 0.$$

In view of the nonsingularity of the matrix X, it follows that $U^+U = I$, i.e., the matrix U is unitary.

We simultaneously see how the unitary matrix U labeling an s.a. extension $\hat{f}_U$ of the symmetric operator $\hat{f}$ is uniquely restored from a given set of vectors $\{w_k\}_1^m$ under a certain choice of the orthogonal bases $\{e_{\pm,k}\}_1^m$ in the respective deficient subspaces $D_\pm$ of $\hat{f}$.

We formulate the results of the above consideration as a supplement to the main theorem; this supplement is the promised modification of the main theorem in its part associated with (3.35).

Theorem 4.18 (Supplement to the main theorem). *Any s.a. extension $\hat{f}_U$ of a symmetric operator $\hat{f}$ with finite equal nonzero deficiency indices, $m_\pm = m$, $0 < m < \infty$, can be defined as*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\xi_U : \xi_U \in D_{f^+};\ \omega_{f^+}(w_k, \xi_U) = 0,\ \forall k\right\}, \\ \hat{f}_U \xi_U = \hat{f}^+ \xi_U, \end{cases} \tag{4.86}$$

where $\{w_k\}_1^m$ is a certain set of vectors belonging to the domain D_{f^+}, $w_k \in D_{f^+}$, linearly independent modulo the domain $D_{\overline{f}}$, and satisfying relations (4.85). Conversely, any set $\{w_k\}_1^m$ of vectors belonging to D_{f^+}, linearly independent modulo $D_{\overline{f}}$, and satisfying relations (4.85) defines a certain s.a. extension of the symmetric operator $\hat{f}$ by (4.86).

Remark 4.19. We note that the $U(m)$-nature of the set $\{\hat{f}_U\}$ of all s.a. extensions proves to be hidden in this formulation of the main theorem. This manifests itself in the fact that the two sets $\{w_k\}_1^m$ and $\{\tilde{w}_k\}_1^m$ of vectors related by a linear transformation $\tilde{w}_k = \sum_{l=1}^m Z_{lk} w_l$, where the matrix $Z = \|Z_{lk}\|$ is nonsingular, define the same s.a. extension. We can say that the description of s.a. extensions according to the supplement to the main theorem is a description with a certain "excess" that is inessential, but controlled.

An application of the supplement to the main theorem to differential operators in $L^2(a, b)$ results in an evident modification of Theorem 4.13.

Theorem 4.20. *Any s.a. extension $\hat{f}_U$ of the initial symmetric operator $\hat{f}$ associated with an s.a. differential operation $\check{f}$ on an interval (a, b) and having equal* *nonzero deficiency indices, $m_{\pm} = m > 0$, can be specified by s.a. boundary conditions as follows:*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{ \psi_U : \psi_U \in D^*_{\check{f}}(a,b),\ [w_k, \psi_U]_f(x)\Big|_a^b = 0,\ \forall k \right\}, \\ \hat{f}_U \psi_U = \check{f}_U, \end{cases} \tag{4.87}$$

where $\{w_k\}_1^m$ is a certain set of functions belonging to the domain D_{f+}, $w_k \in D^*_{\check{f}}(a,b)$, linearly independent modulo the domain $D_{\overline{f}}$ and satisfying the relations

$$[w_k, w_l]_f(x)\Big|_a^b = 0,\ k, l = 1, \ldots, m. \tag{4.88}$$

Conversely, any set $\{w_k\}_1^m$ of functions belonging to D_{f+}, linearly independent modulo $D_{\overline{f}}$, and satisfying relations (4.88) defines a certain s.a. extension of $\hat{f}$ given by (4.87).

Remark 4.19 following the supplement to the main theorem is completely applicable to Theorem 4.20.

Theorem 4.20 yields a modified version of Theorem 4.15 related to regular differential operations. The modification consists in the replacement of the matrices $E_U(a/b)$ (4.67) by the similar $n \times n$ matrices $W(a/b)$ with the matrix elements $W_{lk}(a/b) = w_k^{[l-1]}(a/b)$ generated by the functions $w_k \in D^*_{\check{f}}(a,b)$, $k = 1, \ldots, n$, satisfying the conditions of Theorem 4.20. These conditions, the linear independence of the functions w_k modulo $D_{\overline{f}}$, and relations (4.88) are equivalent to the following two conditions on the matrices $W(a/b)$:

(1) The rank of the rectangular $2n \times n$ matrix $\mathbb{W}$ composed of the two matrices $W(a/b)$ is maximum,

$$\mathbb{W} = (W(a) \diagup W(b)),\ \operatorname{rank}\mathbb{W} = n. \tag{4.89}$$

This property is a complete analogue of (4.70).

(2) The relation

$$W^+(b)\,\mathcal{E}W(b) = W^+(a)\,\mathcal{E}W(a) \tag{4.90}$$

holds, which is an analogue of relation (4.71).

The proof of the necessity of (4.89) is by contradiction. Let $\operatorname{rank}\mathbb{W} < n$. This means that there exists a set $\{c_k\}_1^n$ of numbers such that at least one of them is different from zero, and

$$\sum_{k=1}^{n} W_{lk}(a/b)\,c_k = \sum_{k=1}^{n} w_k^{[l-1]}(a/b)\,c_k = 0.$$

The representation (4.54) then implies that the function $w = \sum_{k=1}^{n} c_k w_k$ belongs to the domain $D_{\overline{f}}$ of the closure $\overline{\hat{f}}$ of $\hat{f}$, which contradicts the linear independence of the functions w_k modulo $D_{\overline{f}}$ unless all c_k are equal to zero. In fact, we here repeat the arguments leading to (4.70).

Conversely, let $W(a/b)$ be two arbitrary matrices satisfying condition (4.89). Because the functions belonging to $D^*_{\check{f}}(a,b)$ and their $n-1$ quasiderivatives can take arbitrary values at the regular endpoints a and b, there exists a set $\{w_k\}_1^n$ of functions $w_k \in D^*_{\check{f}}(a,b)$ such that $W_{lk}(a/b) = w_k^{[l-1]}(a/b)$. These functions are evidently linearly independent modulo $D_{\overline{f}}$.

As to relation (4.90), it is equivalent to relation (4.88) in view of representation (4.14) for the local form $[.,.]_f$ generated by even s.a. differential operations and its modification in terms of the matrix $\mathcal{E}$ (4.66), which were already used before in deducing (4.65) and (4.71). This relation is a direct generalization of relation (4.71). Because the functions w_k are represented in this context only by the boundary values of their quasiderivatives of order from 0 up to $n-1$, it is natural to introduce the notation $A = \|a_{lk}\| = W(a)$, $B = \|b_{lk}\| = W(b)$ and to formulate a modified version of Theorem 4.15 as follows.

Theorem 4.21. *Any s.a. extension $\hat{f}_U$ of the initial symmetric operator $\hat{f}$ associated with a regular even s.a. differential operation $\check{f}$ of order n on an interval (a,b) can be specified by s.a. boundary conditions as follows:*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\psi_U : \psi_U \in D^*_{\check{f}}(a,b);\ B^+\mathcal{E}\Psi_U(b) = A^+\mathcal{E}\Psi_U(a)\right\}, \\ \hat{f}_U\psi_U = \check{f}\psi_U, \end{cases} \tag{4.91}$$

where A and B are some $n \times n$ matrices satisfying the conditions

$$\operatorname{rank}(A/B) = n,\ B^+\mathcal{E}B = A^+\mathcal{E}A, \tag{4.92}$$

the matrix $\mathcal{E}$ and columns $\Psi_U(a/b)$ are defined respectively by (4.66) and (4.68). Conversely, any two matrices A and B satisfying conditions (4.92) define a certain s.a. extension of $\hat{f}$ given by (4.91).

A similar theorem, appropriately modified, holds for any regular s.a. differential operations with the replacement of quasiderivatives by ordinary derivatives because the corresponding boundary forms are finite forms in the boundary values of functions and their derivatives; see Lemma 4.23.

We can also add that the matrices $\tilde{A} = AZ$ and $\tilde{B} = BZ$, where the $n \times n$ matrix Z is nonsingular, define the same s.a. operator. This remark is related to the hidden $U(n)$-nature of s.a. boundary conditions (4.91) and is similar to Remark 4.19 following Theorems 4.18.

In fact, this arbitrariness in the choice of the matrices A and B is unremovable only if their ranks are not maximum,[30] $\operatorname{rank} A < n$, $\operatorname{rank} B < n$ (it follows from condition (4.92) that the matrices A and B are singular or nonsingular simultaneously). If these matrices are nonsingular, which is a generic situation, the indicated arbitrariness can be removed. Indeed, let $\det B \neq 0$, and therefore, $\det A \neq 0$ as well. Then, in view of the property $\mathcal{E}^{-1} = -\mathcal{E}$ of the nonsingular matrix $\mathcal{E}$, s.a. boundary conditions (4.91) can be written as

$$\Psi(b) = S\Psi(a), \ \Psi(a) = S^{-1}\Psi(b), \tag{4.93}$$

where the nonsingular matrix S is given by $S = -\mathcal{E}\left(AB^{-1}\right)^{+}\mathcal{E}$. Because the matrix $\mathcal{E}$ is anti-Hermitian, $\mathcal{E}^{+} = -\mathcal{E}$, the conjugate matrix S^{+} is given by $S^{+} = -\mathcal{E}\left(AB^{-1}\right)\mathcal{E}$, and the second condition in (4.92) is written in terms of S as

$$S^{+}\mathcal{E}S = \mathcal{E}. \tag{4.94}$$

Otherwise, the matrix S is arbitrary.

The algebraic sense of relation (4.94) is clear: this relation implies that the linear transformations $\Psi \longmapsto S\Psi$ defined in an n-dimensional space of n-component columns Ψ with components ψ_l, $l = 1, \ldots, n$, preserve the Hermitian sesquilinear form $(1/i)\Upsilon^{+}\mathcal{E}\Psi$, where Υ is a column with components χ_l, $l = 1, \ldots, n$, or equivalently, preserve the Hermitian quadratic form $(1/i)\Psi^{+}\mathcal{E}\Psi$. The Hermitian matrix $-i\mathcal{E}$ can be easily diagonalized by a unitary transformation:

$$-i\mathcal{E} = T^{+}\Sigma_3 T, \tag{4.95}$$

where the diagonal $n \times n$ matrix Σ_3 equals $\operatorname{diag}(I, -I)$, where I is the $n/2 \times n/2$ identity matrix, and the unitary $n \times n$ matrix $T = \|T_{lm}\|$ is given by

$$\sqrt{2}T_{lm} = \delta_{l,m}\left[\theta(-k) - i\theta(k)\right] + \delta_{l,n+1-m}\left[\theta(-k) + i\theta(k)\right],$$

$$k = m - (n+1)/2, \tag{4.96}$$

where $\theta(x)$ is the well-known step function. The signature of the matrix $(1/i)\mathcal{E}$ is equal to $(n/2, n/2)$, which implies that the transformations S satisfying condition (4.94) form the group $U(n/2, n/2)$. We thus obtain that in the generic case, the s.a. boundary conditions are parameterized by elements of the group $U(n/2, n/2)$, which defines an embedding of the group $U(n/2, n/2)$ into the group $U(n)$ that parameterizes all possible s.a. boundary conditions. This embedding is an embedding "into," but not "onto": although both $U(n/2, n/2)$ and $U(n)$ are n^2-parameter manifolds, the group $U(n/2, n/2)$ is noncompact, whereas the group $U(n)$ is compact; it is also clear from the above discussion that s.a. boundary conditions (4.91) cannot be represented in the form (4.93) if the matrices A and

[30] Of course, this condition is compatible with condition (4.92).

B are singular. In the latter case, the boundary conditions can be obtained from (4.93) by a certain limiting process whereby some matrix elements of the matrix S tend to infinity, while some others tend to zero (we note that $|\det S| = 1$). This process corresponds to a compactification of the group $U(n/2, n/2)$ to the group $U(n)$ by adding some limit elements.

It is worth noting that in looking at the representation of the asymmetry form ω_{f^+} in terms of the boundary values of functions and their quasiderivatives in the case of regular even s.a. differential operations,[31]

$$\omega_{f^+}(\chi_*, \psi_*) = \Upsilon_*^+(b)\mathcal{E}\Psi_*(b) - \Upsilon_*^+(a)\mathcal{E}\Psi_*(a), \tag{4.97}$$

where the n-component columns $\Upsilon_*(a), \Upsilon_*(b)$ and $\Psi_*(a), \Psi_*(b)$ are defined by (4.68) under the respective changes $\psi_U \to \chi_*$ and $\psi_U \to \psi_*$, we can easily see from the very beginning that boundary conditions (4.93) with any fixed matrices S satisfying condition (4.94) result in the vanishing of the asymmetry form ω_{f^+} and thus define a symmetric restriction of the adjoint operator $\hat{f}^+$. Using the standard technique of evaluating the adjoint operator in terms of the asymmetry form ω_{f^+}, see Sect. 3.2, it is easy to prove that boundary conditions (4.93) and (4.94) are actually s.a. boundary conditions defining an s.a. restriction of the operator $\hat{f}^+$. Unfortunately, they do not exhaust all possible s.a. boundary conditions.

It may be instructive to illustrate Theorem 4.21 and also s.a. boundary conditions (4.93) and (4.94) by our favorite example of the regular second-order s.a. differential operation $\check{\mathcal{H}}$ (4.7) on an interval $[0, l]$. Our goal is to show how already known s.a. boundary conditions (4.72)–(4.75) are obtained without evaluating the deficient subspaces.

Let now $A = \|\delta_{i2}\delta_{j2}\|$ and $B = \|\delta_{i2}\delta_{j1}\|$. It is easy to verify that these matrices satisfy conditions (4.92); then (4.91) yields the s.a. boundary conditions $\psi(0) = \psi(l) = 0$ coinciding with (4.73). These boundary conditions can be obtained from (4.93) with the matrix $S(\varepsilon) = \operatorname{antidiag}(1/\varepsilon, -\varepsilon)$ by passing to the limit $\varepsilon \to 0$. Such a matrix $S(\varepsilon)$ arises if we slightly deform the initial matrices A and B, $A \to A(\varepsilon) = \operatorname{diag}(\varepsilon, 1)$ and $B \to B(\varepsilon) = \operatorname{antidiag}(1, -\varepsilon)$, removing their singularity without breaking conditions (4.92).

Let now $A = \|\delta_{i1}\delta_{j2}\|$ and $B = \|\delta_{i1}\delta_{j1}\|$. These matrices also satisfy conditions (4.92); then (4.91) yields the s.a. boundary conditions $\psi'(0) = \psi'(l) = 0$ coinciding with (4.74). Again, these boundary conditions can be obtained from (4.93) with the matrix $S(\varepsilon) = \operatorname{antidiag}(\varepsilon, -1/\varepsilon)$ by passing to the limit $\varepsilon \to 0$. The matrix $S(\varepsilon)$ arises as a result of the deformation $A \to A(\varepsilon) = \operatorname{antidiag}(-\varepsilon, 1)$, and $B \to B(\varepsilon) = \operatorname{diag}(1, \varepsilon)$.

If we choose $A = \|a_2\delta_{i1}\delta_{j2} + a_4\delta_{i2}\delta_{j2}\|$ and $B = \|b_1\delta_{i1}\delta_{j1} + b_3\delta_{i2}\delta_{j1}\|$, where at least one of the numbers in the pairs a_2, a_4 and b_1, b_3 is different from zero, which is required by the first of conditions (4.92), and in addition $a_2\overline{a_4} = \overline{a_2}a_4$ and

[31] In fact, this representation based on (4.14), (4.34) and (4.35), could have been cited much earlier, at least at the beginning of the above consideration leading to (4.65)–(4.71).

$b_1\overline{b_3} = \overline{b_1}b_3$, which is required by the second of conditions (4.92), we obtain the so-called *split s.a. boundary conditions*

$$\psi'(0) = \lambda\psi(0), \ \psi'(l) = \mu\psi(l),$$

where $\lambda = \overline{a_4}/\overline{a_2} = a_4/a_2$, $\mu = \overline{b_3}/\overline{b_1} = b_3/b_1 \in \overline{\mathbb{R}}$, so that $\lambda = \pm\infty$ yield the same boundary condition $\psi(0) = 0$, and $\mu = \pm\infty$ yield the same boundary condition $\psi(l) = 0$.

Setting $S = I$ in (4.93), we obtain the periodic boundary conditions $\psi(0) = \psi(l)$, $\psi'(0) = \psi'(l)$, coinciding with (4.75). But if we choose $S = e^{i\vartheta}I$, $\vartheta \in \mathbb{S}(0, 2\pi)$, we obtain the modified periodic boundary conditions $\psi(l) = e^{i\vartheta}\psi(0)$, $\psi'(l) = e^{i\vartheta}\psi'(0)$, which include both periodic, $\vartheta = 0$, and antiperiodic, $\vartheta = \pi$, boundary conditions.

As to the "mixed" s.a. boundary conditions (4.72), it is easy to verify that they can be represented in the form (4.93), $\Psi(l) = S\Psi(0)$, with the matrix

$$S = -\begin{pmatrix} \cosh\pi & l\pi^{-1}\sinh\pi \\ \pi l^{-1}\sinh\pi & \cosh\pi \end{pmatrix},$$

satisfying condition (4.94).

Theorem 4.20 also provides a modified version of Theorem 4.17 that is obtained by reasoning completely similar to the previous one.

Theorem 4.22. *Let $\check{f}$ be an even s.a. differential operation of order n on an interval (a, b) with a regular endpoint a and a singular endpoint b, and let the associated initial symmetric operator $\hat{f}$ have the minimum possible deficiency indices $m_\pm = n/2$, which is equivalent to the triviality of the (right) boundary form at the singular endpoint b. Then any s.a. extension $\hat{f}_U$ can be specified by s.a. boundary conditions as follows:*

$$\hat{f}_U : \begin{cases} D_{f_U} = \left\{\psi_U : \psi_U \in D^*_{\check{f}}(a, b), \ A^+_{1/2}\mathcal{E}\psi_U(a) = 0\right\}, \\ \hat{f}_U\psi_U = \check{f}\psi_U, \end{cases} \tag{4.98}$$

where $A_{1/2}$ is a rectangular $n \times n/2$ matrix satisfying the conditions

$$\operatorname{rank} A_{1/2} = n/2, \ A^+_{1/2}\mathcal{E}A_{1/2} = 0, \tag{4.99}$$

and the matrix $\mathcal{E}$ and column $\Psi_U(a)$ are defined respectively by (4.66) and (4.68). Conversely, any $n \times n/2$ matrix A satisfying conditions (4.99) defines a certain s.a. extension of $\hat{f}$ given by (4.98). If the endpoint a is singular, while the endpoint b is regular, $A_{1/2}$ and a in (4.98) and (4.99) are respectively exchanged for $B_{1/2}$ and b.

Similar to Theorem 4.21, this theorem can be supplemented with a remark about a hidden $U(n/2)$-nature of s.a. boundary conditions (4.98): the matrices $A_{1/2}$ and $A_{1/2}Z$, where Z is any nonsingular $n/2 \times n/2$ matrix, yield the same s.a. operator.

We illustrate this theorem by the example of s.a. differential operation $\check{\mathcal{H}}$ (4.7) of order $n = 2$ on the semiaxis $\mathbb{R}_+$. This differential operation satisfies the conditions of Theorem 4.22, as well as of Theorem 4.17: the left endpoint $a = 0$ is evidently regular, the right endpoint b is singular, but the boundary form at the singular endpoint is trivial, $[.,.]_{\mathcal{H}}(\infty) = 0$, by Lemma 2.14 (we already mentioned this fact in Sect. 4.3 when we considered $\check{\mathcal{H}}$ on the whole axis).[32]

Again, our aim is to demonstrate how s.a. operators associated with $\check{\mathcal{H}}$ on $\mathbb{R}_+$ can be constructed and specified without evaluating the deficient subspaces of the initial symmetric operator $\widehat{\mathcal{H}}$. The matrix $A_{1/2}$ in the case of $n = 2$ is a column of two numbers a_1, a_2 at least one of which is different from zero, which is required by the first of conditions (4.99), while the second of conditions (4.99) requires that the equality $\overline{a_1}a_2 = a_1\overline{a_2}$ be fulfilled. Formula (4.98) with $\check{f} = \check{\mathcal{H}}$ then defines a one-parameter family $\widehat{\mathcal{H}}_\lambda$, $\lambda \in \overline{\mathbb{R}}$, of s.a. operators $\widehat{\mathcal{H}}_\lambda$ associated with $\check{\mathcal{H}}$ and specified by the s.a. boundary conditions $\psi'(0) = \lambda\psi(0)$, $\lambda = \overline{a_2}/\overline{a_1} = a_2/a_1$; see also Sect. 6.2. It is evident that the same s.a. boundary conditions specify the s.a. operators $\hat{H}_\lambda$ associated with the s.a. differential operation $\check{H} = \check{\mathcal{H}} + V(x)$ (4.8) on the semiaxis $\mathbb{R}_+$ in the case that the potential is bounded, $|V(x)| < M$; an operator $\hat{H}_\lambda$ is defined on the same domain as an operator $\widehat{\mathcal{H}}_\lambda$. The same s.a. boundary conditions holds also for a set of unbounded potentials. See Sect. 7.1.

4.7 Asymmetry Form Method for Specifying Self-adjoint Extensions in Terms of Explicit Self-adjoint Boundary Conditions

The above-presented traditional methods for constructing s.a. operators associated with s.a. differential operations as s.a. extensions of the initial symmetric operators and their specification in terms of s.a. boundary conditions do not always provide an explicit form of these conditions, especially in the presence of singular endpoints, so that the $U(m)$-nature of the whole family of the associated s.a. operators is not evident.

We now discuss another possible method, additional to the traditional ones, for specifying the associated s.a. differential operators in terms of explicit, generally asymptotic, s.a. boundary conditions; the $U(m)$-nature of this description is evident. For brevity, we call this method the *asymmetry form method*. The idea of this method is based on two observations. Both observations equally concern the asymmetry forms ω_{f+} and Δ_{f+}. It is more convenient for us to deal with the quadratic asymmetry form Δ_{f+}, although all that is stated below is applicable to the sesquilinear asymmetry form ω_{f+} as well: we recall that the forms Δ_{f+} and

[32]It is also easy to verify that the deficiency indices of the initial symmetric operator $\widehat{\mathcal{H}}$ are minimum, $m_\pm = n/2 = 1$ (see Sect. 6.2).

ω_{f+} determine each other; see Sect. 3.2. This section is comparatively independent of the previous section, and for its completeness, we cite some basic notions.

The first observation is as follows. For ordinary differential operators, it is convenient to represent finite-dimensional deficient subspaces $D_\pm$ (4.43) in terms of their orthogonal decompositions (4.47), i.e., to represent deficient vectors $\psi_\pm$ in terms of their expansion coefficients $c_{\pm,k}$, which are dimensionless by definition. Namely, under a certain choice (arbitrary, but fixed) of the orthogonal basis $\{e_{\pm,k}\}_1^{m\pm}$ in $D_\pm$, the deficient subspaces D_+ and D_- can be identified with the respective finite-dimensional Euclidean linear spaces $\mathbb{C}_+^{m+}$ of m_+-component columns $\{c_{+,k}\}_1^{m+}$ and $\mathbb{C}_-^{m-}$ of m_--component columns $\{c_{-,k}\}_1^{m-}$, $D_+ \Leftrightarrow \mathbb{C}_+^{m+}$ and $D_- \Leftrightarrow \mathbb{C}_-^{m-}$. In this representation, the quadratic asymmetry form, which is defined on the natural domain $D^*_{\check{f}}(a,b) = D_{f+} = D_{\overline{f}} + D_+ + D_-$, but is nontrivial only on $D_+ + D_-$, becomes

$$\Delta_{f+}(\psi_*) = 2\mathrm{i}\kappa\left(\sum_{k=1}^{m+}|c_{+,k}|^2 - \sum_{k=1}^{m-}|c_{-,k}|^2\right), \tag{4.100}$$

or the quadratic form $(1/2\mathrm{i}\kappa)\Delta_{f+}$ becomes a canonical diagonal Hermitian form in the complex linear space $\mathbb{C}^{m_++m_-} = \mathbb{C}_+^{m+} + \mathbb{C}_-^{m-}$, the direct sum[33] of the spaces $\mathbb{C}_+^{m+}$ and $\mathbb{C}_-^{m-}$ giving contributions of opposite signs to the quadratic form. The deficiency indices $m_\pm$ determine the signature of this quadratic form, $\mathrm{sgn}\,(1/2\mathrm{i}\kappa)\Delta_{f+} = (m_+, m_-)$, and manifest themselves as its inertia indices; we recall that $m_\pm \le n$, where n is the order of the differential operation $\check{f}$; see Sect. 4.4. For brevity, we call representation (4.100) the *canonical diagonal form* for Δ_{f+} and call m_+, m_- its inertia indices, by this is actually the form $(1/2\mathrm{i}\kappa)\Delta_{f+}$.

We can examine the problem of symmetric and s.a. extensions of the initial symmetric operator $\hat{f}$ in terms of the expansion coefficients $c_{\pm,k}$. We can repeat all the arguments in Sects. 3.3 and 3.4 resulting in the main theorem with the same conclusions in these terms. In particular, if the inertia indices are equal, $m_\pm = m$, the isometries $\hat{U} : \mathbb{C}_+^m \longmapsto \mathbb{C}_-^m$ that are directly given by unitary $m \times m$ matrices U provide the vanishing of the forms Δ_{f+} and ω_{f+} and thereby produce the m^2-parameter family $\{\hat{f}_U, U \in U(m)\}$ of s.a. extensions of the initial symmetric operator $\hat{f}$.

We now observe that we can choose an arbitrary mixed basis $\{e_k\}_1^{m_++m_-}$ in the direct sum $D_+ + D_-$ such that

$$\psi_+ + \psi_- = \sum_{k=1}^{m_++m_-} c_k e_k. \tag{4.101}$$

[33] We recall that this sum is direct, but not orthogonal.

Correspondingly, the basis in $\mathbb{C}^{m_+ + m_-}$ also changes, and the form Δ_{f+} becomes

$$\Delta_{f+}(\psi_*) = 2\mathrm{i}\kappa \sum_{k,l=1}^{m_+ + m_-} \overline{c_k}\omega_{kl}c_l, \tag{4.102}$$

where $(m_+ + m_-)\times(m_+ + m_-)$ matrix $\omega = \|\omega_{kl}\|$ is dimensionless and Hermitian, $\omega_{kl} = \overline{\omega_{lk}}$, or $(1/2\mathrm{i}\kappa)\Delta_{f+}$ becomes a general Hermitian quadratic form, of course of the same signature. We can reduce representation (4.102) to canonical diagonal form (4.100) in a standard way[34] and repeat the already known arguments with the same conclusions.

The second observation includes some suggestions. In the case of differential operators, the quadratic asymmetry form Δ_{f+} is expressed in terms of the quadratic boundary forms, the boundary values of the quadratic local form $[\psi_*, \psi_*]_f(x)$ in functions and their (quasi)derivatives; see representations (4.36) and (4.37). We know that for an even s.a. differential operation $\check{f}$ of order n, the boundary forms, both sesquilinear and quadratic, at a regular endpoint are finite nontrivial forms of order n in finite boundary values of functions and their quasiderivatives of order up to $n-1$, see (4.14), which considerably simplified the analysis of s.a. boundary conditions in the previous section. More specifically, let the left endpoint a of the interval be regular. As is evident from representation (4.97) for the sesquilinear form ω_{f+} in terms of boundary forms, the left quadratic boundary form $[\psi_*, \psi_*]_f(a)$ is represented as

$$[\psi_*, \psi_*]_f(a) = \Psi_*^+(a)\mathcal{E}\Psi_*(a), \tag{4.103}$$

where the n-column $\Psi_*(a)$ is given by (4.68) with the change of subscript $U \to *$, and the $n \times n$ matrix $\mathcal{E}$ is given by (4.66). Of course, a similar representation holds for the right boundary form $[\psi_*, \psi_*]_f(b)$ if the right endpoint b is regular.

To our knowledge, the notion of quasiderivatives and similar assertions are absent for odd and mixed s.a. differential operations. However, we can prove the following lemma.

Lemma 4.23. *For any s.a. differential operation of finite order, the sesquilinear and quadratic boundary forms at a regular endpoint are finite forms in the respective boundary values of functions and their derivatives of order up to* $n-1$.

Proof. According to (4.13), the anti-Hermitian sesquilinear local form

$$[\chi_*, \psi_*]_f(x)$$

[34]The so-called reduction to the principal axes of inertia by invertible linear transformations of the expansion coefficients.

for an s.a. differential operation $\check{f}$ of order n on an interval (a, b) allows the representation

$$[\chi_*, \psi_*]_f\,(x) = i \sum_{k,l=1}^{n} \overline{\chi_*^{(k)}}(x)\, \widetilde{\omega}_{kl}(x)\, \psi_*^{(l)}(x) \tag{4.104}$$

inside the interval, where the Hermitian $n \times n$ matrix $\widetilde{\omega}(x) = \|\widetilde{\omega}_{kl}(x)\|$ is continuous. We prove that this matrix has a finite limit at a regular endpoint, i.e., it is continuous up to a regular endpoint. For brevity, we speak about continuity at a regular endpoint. The proof is based on the continuity of the sesquilinear local form $[\chi_*, \psi_*]_f\,(x)$ at any endpoint and the continuity of functions $\psi_*^{(k-1)}(x)$, $k = 1, \ldots, n$, at a regular endpoint. Let the left endpoint a be a regular endpoint. We take a collection of functions $\psi_{*\alpha}(x)$, $\alpha = 1, \ldots, n$, so that the $n \times n$ matrix $\Psi(x) = \left\|\psi_{*\alpha}^{(k-1)}(x)\right\|$, which is continuous at the left endpoint a, is nonsingular on an interval $[a, a + \epsilon]$, where ϵ is sufficiently small.[35] We then consider the $n \times n$ matrix $\Omega(x) = [\psi_{*\alpha}, \psi_{*\beta}]_f(x)$. According to (4.104), this matrix allows the representation

$$\Omega(x) = \Psi^+(x)\widetilde{\omega}(x)\Psi(x),\ \Psi^+(x) = (\Psi(x))^+,$$

inside the interval, whence follows the representation

$$\widetilde{\omega}(x) = (\Psi^+(x))^{-1}\Omega(x)\,(\Psi(x))^{-1}$$

for the matrix $\widetilde{\omega}(x)$. Because all the matrices on the right-hand side of this representation are continuous at the regular endpoint a, the matrix $\widetilde{\omega}(x)$ is also continuous at this endpoint, i.e., the matrix $\widetilde{\omega}(a)$ exists and is finite. This means that representation (4.104) can be extended to $x = a$, i.e., to the left sesquilinear boundary form $[\chi_*, \psi_*]_f\,(a)$ and therefore to its reduction to the diagonal, the quadratic boundary form $[\psi_*, \psi_*]_f\,(a)$. Similar arguments are applicable to the right regular endpoint b, which completes the proof of the lemma. □

This lemma allows considering even and noneven s.a. differential operations $\check{f}$ on an equal footing. The only difference is that derivatives for the general $\check{f}$ are replaced by quasiderivatives for even $\check{f}$.

Because the boundary values of functions and their (quasi)derivatives are generally dimensional, it is convenient to introduce dimensionless quantities c_k coinciding with derivatives $\psi_*^{(k-1)}$, or quasiderivatives $\psi_*^{[k-1]}$ for even $\check{f}$, at a regular endpoint up to a corresponding dimensional factor. It is also convenient to redefine the dimensional matrix elements $\widetilde{\omega}_{kl}(a/b)$, if they occur, by a dimensional

[35] For example, we can take functions $\psi_{*\alpha}$ such that $\psi_{*\alpha}^{(k-1)}(x_0) = \delta_\alpha^k$, $x_0 \in [a, a + \epsilon]$.

factor, $\widetilde{\omega}_{kl}(a/b) \to \omega_{kl}(a/b)$, where $\omega_{kl}(a/b)$ are dimensionless.[36] Then the left quadratic boundary form for an s.a. differential operation $\check{f}$ of order n with a regular endpoint a becomes[37]

$$[\psi_*, \psi_*](a) = 2\mathrm{i}\kappa \sum_{k,l=1}^{n} \overline{c_k(a)}\omega_{kl}(a)c_l(a), \;\; \omega_{kl}(a) = \overline{\omega_{lk}(a)}, \tag{4.105}$$

where $c_k(a)$, $k = 1, \dots, n$, are boundary values of (quasi)derivatives of ψ_* of respective orders $0, 1, \dots, n-1$ at the left endpoint a up to some arbitrary, but fixed, dimensional factor, its own for each k, so that all $c_k(a)$ are dimensionless, the Hermitian $n \times n$ matrix $\omega(a) = \|\omega_{kl}(a)\|$ is also dimensionless, and κ is a common dimensional factor of the dimension of $\check{f}$. The common dimensional factor $2\mathrm{i}\kappa$ is extracted for the convenience of further comparisons. In principle, the number $p(a)$ of essential parameters $c_k(a)$ in (4.105) could be less than n if the matrix $\omega_{kl}(a)$ were singular, i.e., $\operatorname{rank}\omega(a) < n$, but we show below that $p(a) = n$, or $\operatorname{rank}\omega(a) = n$ for a regular endpoint.[38]

A similar representation holds for the right boundary form $[\psi_*, \psi_*](b)$ if the right endpoint b is regular:

$$[\psi_*, \psi_*](b) = 2\mathrm{i}\kappa \sum_{k,l=1}^{n} \overline{c_k(b)}\omega_{kl}(b)c_l(b), \omega_{kl}(b) = \overline{\omega_{lk}(b)}, \tag{4.106}$$

with a similar meaning of the quantities $c_k(b)$, $k = 1, \dots, n$, and a dimensionless Hermitian $n \times n$ matrix $\omega(b) = \|\omega_{kl}(b)\|$. Again, the number $p(b)$ of essential parameters $c_k(b)$ is equal to n, or $\operatorname{rank}\omega(b) = n$.

For a singular endpoint where the functions belonging to $D^*_{\check{f}}(a,b)$ and their (quasi)derivatives can have singularities, an evaluation of the corresponding boundary form, which is certainly finite, is generally nontrivial. Our suggestion is that the quadratic boundary form at a singular endpoint is a quadratic form in finite dimensionless coefficients of asymptotic expansions of the functions belonging to $D^*_{\check{f}}(a,b)$ at the endpoint. More specifically, let the left endpoint a be singular for an s.a. differential operation $\check{f}$ of order n. We assume that the asymptotic behavior of the functions belonging to $D^*_{\check{f}}(a,b)$ at this endpoint can be represented as

$$\psi_*(x) = \sum_{k=1}^{p(a)} c_k(a)\psi_{\mathrm{as}\,k}(a,x) + \widetilde{\psi}_{\mathrm{as}}(a,x), \;\; x \to a, \tag{4.107}$$

[36]We clarify this point below by the example of a regular even s.a. differential operation.

[37]From this point on, we omit the subscript f in the symbol of boundary forms.

[38]For even s.a. differential operations, this is evident from (4.103).

the sum of leading asymptotic summands $\sum_{k=1}^{p(a)} c_k(a)\psi_{\text{as}k}(a,x)$ and an irrelevant summand $\widetilde{\psi}_{\text{as}}(a,x)$; the (quasi)derivatives of order up to $n-1$ for $\psi_*(x)$ are given by directly differentiating representation (4.107). The functions $\psi_{\text{as}\,k}(a,x)$ are linearly independent functions, generally singular together with their (quasi)derivatives as $x \to a$, that give finite contributions to the left quadratic boundary form $[\psi_*,\psi_*](a)$, so that this form is a finite quadratic form in the independent dimensionless coefficients $c_k(a),\ k=1,\dots,p(a)$, of asymptotic expansion (4.107):

$$[\psi_*,\psi_*](a) = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(a)} \overline{c_k(a)}\omega_{kl}(a)c_l(a),\ \omega_{kl}(a) = \overline{\omega_{lk}(a)}, \tag{4.108}$$

where the Hermitian $p(a)\times p(a)$ matrix $\omega(a) = \|\omega_{kl}(a)\|$ is dimensionless. This representation of the left quadratic boundary form for a singular endpoint is similar to representation (4.105) for a regular endpoint, but the meaning of the coefficients $c_k(a)$ and matrix elements $\omega_{kl}(a)$ is different, in particular, generally $p(a)\neq n$. The functions $\psi_{\text{as}\,k}(a,x)$, $k=1,\dots,p(a)$, in particular, their number $p(a)$, are specific for a given singular $\check{f}$. We show below that $p(a)\leq n$. The functions $\widetilde{\psi}_{\text{as}}(a,x)$ give no contribution to the left boundary form. Representations similar to (4.107) and (4.108) with the change $a\to b$,

$$\psi_*(x) = \sum_{k=1}^{p(b)} c_k(b)\psi_{\text{as}\,k}(b,x) + \widetilde{\psi}_{\text{as}}(b,x),\ x\to b, \tag{4.109}$$

$$[\psi_*,\psi_*](b) = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(b)} \overline{c_k(b)}\omega_{kl}(b)c_l(b),\ \omega_{kl}(b) = \overline{\omega_{lk}(b)}, \tag{4.110}$$

hold for the singular endpoint b. The functions $\psi_{\text{as}\,k}(a,x)$ and $\psi_{\text{as}\,k}(b,x)$, their numbers $p(a)$ and $p(b)$, and the matrices $\omega(a)$ and $\omega(b)$ are generally different. If the left or/and right boundary form is trivial, i.e., is identically zero,[39] we respectively set $p(a)=0$ or/and $p(b)=0$.

We thus obtain that in the general case, the quadratic boundary forms are expressed in terms of the dimensionless coefficients proportional to the boundary values of functions belonging to $D^*_{\check{f}}(a,b)$ and their (quasi)derivatives (the case of a regular endpoint) and/or in terms of the dimensionless coefficients c_k of asymptotic expansions (4.107), (4.109) (the case of a singular endpoint). We combine these quantities into one set under the name of *asymptotic boundary coefficients* (*a.b. coefficients* in what follows). Because the boundary forms at different endpoints of the interval (a,b) are independent, see Sect. 4.3, the independent left a.b. coefficients $c_k(a),\ k=1,\dots,p(a)$, and right a.b. coefficients $c_k(b),\ k=1,\dots,p(b)$,

[39] This is possible for a singular endpoint; examples are given below.

are naturally distinguished. As a result, the set $\mathbb{C}^{p(a)}$ of left a.b. coefficients that is the linear space of $p(a)$-component columns $\{c_k(a)\}_1^{p(a)}$ is associated with the left endpoint a, while the (independent) set $\mathbb{C}^{p(b)}$ of right a.b. coefficients that is the linear space of $p(b)$-component columns $\{c_k(b)\}_1^{p(b)}$ is associated with the right endpoint b. If the endpoint a for a given s.a. differential operation $\check{f}$ of order n is regular, then $p(a) = n$, and the same holds for the right endpoint b. The whole number of a.b. coefficients is the sum $p(a) + p(b)$.

At present, we do not know a universal recipe for finding the a.b. coefficients for singular endpoints; a solution of this problem remains a matter of craftsmanship. We can only make a suggestion. Its validity is confirmed by examples considered in subsequent chapters, but its applicability to the general case is not clear now. The suggestion is that the set $\{\psi_{\mathrm{as},k}(x)\}$ of leading asymptotic functions for a singular endpoint is the set of the fundamental solutions of the homogeneous equation $\check{f}u = 0$ that are square-integrable at this endpoint, in other words, the asymptotic behavior of functions ψ_* at the singular endpoint is described by linear combinations of such fundamental solutions. Because of the requirement of square-integrability, the number of a.b. coefficients for a singular endpoint can be less than the order n of $\check{f}$. It may happen that the set of a.b. coefficients for some singular endpoint is empty, in which case the boundary form at this endpoint is trivial.

Let the $(p(a) + p(b))$-component column $\{c_k\}_1^{p(a)+p(b)}$ combine the left and right a.b. coefficients for a function $\psi_*(x)$ belonging to $D^*_{\check{f}}(a, b)$,

$$\{c_k\}_1^{p(a)+p(b)} = \left(\{c_k(a)\}_1^{p(a)} \Big/ \{c_k(b)\}_1^{p(b)}\right).$$

Such columns form the linear space $\mathbb{C}^{p(a)+p(b)} = \mathbb{C}^{p(a)} + \mathbb{C}^{p(b)}$, and the quadratic asymmetry form Δ_{f+} becomes an (anti-Hermitian) quadratic form in this space:

$$\Delta_{f+}(\psi_*) = [\psi_*, \psi_*](x)|_a^b = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(b)} \overline{c_k}(b)\omega_{kl}(b)c_l(b)$$
$$- 2\mathrm{i}\kappa \sum_{k,l=1}^{p(a)} \overline{c_k}(a)\omega_{kl}(a)c_l(a) = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(a)+p(b)} \overline{c_k}\omega_{kl}c_l\,, \qquad (4.111)$$

where the dimensionless $(p(a) + p(b)) \times (p(a) + p(b))$ Hermitian matrix $\omega = \|\omega_{kl}\|$ is block diagonal,

$$\omega = \mathrm{diag}\,(-\omega(a), \omega(b))\,, \qquad (4.112)$$

and the contributions of the right and left a.b. coefficients enter additively.

The representation (4.111) for $\Delta_{f+}(\psi_*)$ can be reduced to a canonical diagonal form[40] in a standard way by invertible linear transformations of a.b. coefficients c_k. Such a reduction can be done separately for the forms $[\psi_*, \psi_*](a)$ and $[\psi_*, \psi_*](b)$ (again, we actually mean the Hermitian forms $(2i\kappa)^{-1}[\psi_*, \psi_*](a)$ and $(2i\kappa)^{-1}[\psi_*, \psi_*](b)$, or the respective Hermitian matrices $\omega(a)$ and $\omega(b)$) by invertible linear transformations of the respective a.b. coefficients $c_k(a)$ and $c_k(b)$ to yield

$$[\psi_*, \psi_*](a) = 2i\kappa \left(\sum_{k=1}^{m_+(a)} |c_{+\,k}(a)|^2 - \sum_{k=1}^{m_-(a)} |c_{-\,k}(a)|^2 \right), \tag{4.113}$$

$$[\psi_*, \psi_*](b) = 2i\kappa \left(\sum_{k=1}^{m_+(b)} |c_{+\,k}(b)|^2 - \sum_{k=1}^{m_-(b)} |c_{-\,k}(b)|^2 \right), \tag{4.114}$$

where $c_{\pm\,k}(a)$ and $c_{\pm\,k}(b)$ are certain linear combinations of the respective a.b. coefficients $c_k(a)$ and $c_k(b)$. It is natural to call these quantities the respective left and right diagonal a.b. coefficients. The integers $m_\pm(a)$ and $m_\pm(b)$ are the inertia indices of the respective boundary forms $[\psi_*, \psi_*](a)$ and $[\psi_*, \psi_*](b)$,

$$m_+(a) + m_-(a) = p(a),\ m_+(b) + m_-(b) = p(b).$$

In terms of the diagonal a.b. coefficients, the quadratic asymmetry form Δ_{f+} becomes

$$\begin{aligned}\Delta_{f+}(\psi_*) = 2i\kappa \Bigg[&\left(\sum_{k}^{m_+(b)} |c_{+\,k}(b)|^2 - \sum_{k=1}^{m_-(b)} |c_{-\,k}(b)|^2 \right) \\ &- \left(\sum_{k}^{m_+(a)} |c_{+\,k}(a)|^2 - \sum_{k=1}^{m_-(a)} |c_{-\,k}(a)|^2 \right) \Bigg] \\ = 2i\kappa &\left(\sum_{k=1}^{m_+(b)+m_-(a)} |c_{+\,k}|^2 - \sum_{l=1}^{m_-(b)+m_+(a)} |c_{-\,k}|^2 \right),\end{aligned} \tag{4.115}$$

where the $(m_+(b) + m_-(a))$-component columns $\{c_+\}_1^{m_+(b)+m_-(a)}$ and $(m_-(b) + m_+(a))$-component columns $\{c_-\}_1^{m_-(b)+m_+(a)}$ of the diagonal a.b. coefficients combine the partial right and left diagonal a.b. coefficients $c_{\pm\,k}(b)$ and $c_{\pm\,k}(a)$ respectively as follows:

[40] We recall that by this, we actually mean the Hermitian form $\frac{1}{2i\kappa}\Delta_{f+}$; this reduction is equivalent to reducing the Hermitian matrix ω to a canonical diagonal form.

$$\{c_{+\,k}\}_1^{m_+(b)+m_-(a)} = \left(\{c_{+\,k}(b)\}_1^{m_+(b)} \Big/ \{c_{-\,k}(a)\}_1^{m_-(a)}\right),$$

$$\{c_{-\,k}\}_1^{m_-(b)+m_+(a)} = \left(\{c_{-\,k}(b)\}_1^{m_-(b)} \Big/ \{c_{+\,k}(a)\}_1^{m_+(a)}\right). \tag{4.116}$$

The inertia indices of Δ_{f+} as the quadratic form in the a.b. coefficients are $m_+(b) + m_-(a)$ and $m_-(b) + m_+(a)$. Of course, there are different, but equivalent, ways of reducing the form Δ_{f+} to a canonical diagonal form with other diagonal a.b. coefficients.

It now suffices to compare representations (4.102) and (4.111) and representations (4.100) and (4.115) of the same quadratic asymmetry form in terms of the quantities c_k and $c_{\pm k}$, the respective expansion coefficients and a.b. coefficients different as to their origin, to reach some important conclusions.

The first conclusion is that the a.b. coefficients must be identified with the expansion coefficients in (4.101) under a certain choice of the basis $\{e_k\}_1^{m_+ + m_-}$ in the direct sum $D_+ + D_-$ of the deficient subspaces; that is why we intentionally let the same letters denote the expansion coefficients and the a.b. coefficients. We can say that in the case of differential operators, the nonzero contributions to the quadratic asymmetry form Δ_{f+}, which owe their existence to the deficient subspaces, are completely determined by the a.b. coefficients for the functions belonging to the natural domain $D^*_{\check{f}}(a,b)$, more exactly, to their $(D_+ + D_-)$-components; it is only the asymptotic behavior of these functions at the boundary of the interval (a,b) that is significant. Correspondingly, the total number of a.b. coefficients is the sum of the deficiency indices,

$$p(a) + p(b) = m_+ + m_-, \tag{4.117}$$

and the signature of Δ_{f+} considered as the quadratic form in a.b. coefficients, see (4.115), determines the deficiency indices $m_\pm$ identifying them with the inertia indices of this form,

$$m_+ = m_+(b) + m_-(a), \;\; m_- = m_-(b) + m_+(a). \tag{4.118}$$

Equality (4.117) allows us to establish certain relations between the numbers $p(a)$ and $p(b)$ of the respective left and right a.b. coefficients, the deficiency indices $m_\pm$, and the order n of a given differential operation. In the general case, we have $m_\pm \le n$ and $m_+ + m_- \le 2n$, so that the total number of a.b. coefficients cannot exceed $2n$, $p(a) + p(b) \le 2n$.

We now show that if the endpoint a is regular, then $p(a) = n$. Let $\check{f}_{a\alpha}$ be the restrictions of the initial s.a. differential operation $\check{f}$ to the interval (a,α), $a < \alpha < b$. It is evident that $\check{f}_{a\alpha}$ is a regular s.a. differential operation of the same order n; therefore the deficiency indices $m_{a\alpha,\pm}$ of the associated initial symmetric operator $\hat{f}_{a\alpha}$ are equal to n. It is also evident that the endpoint α is regular and therefore $p(\alpha) \leq n$. Because $p(a) \leq n$, equality (4.117) (with $b \to \alpha$) yields $p(a) = p(\alpha) = n$. If the endpoint b is regular, we similarly obtain that $p(b) = n$.

Let the endpoint a be singular. Considering the restrictions $\check{f}_{a\alpha}$ of the initial s.a. differential operation $\check{f}$ to the interval (a, α), $a < \alpha < b$, and taking into account equality (4.117) with $b \to \alpha$ and $p(\alpha) = n$ and the inequality $m_{a\alpha,+} + m_{a\alpha,-} \leq 2n$, we obtain that $p(a) \leq n$. If the right endpoint b is singular, similar arguments show that $p(b) \leq n$.

We thus obtain that the number of a.b. coefficients for any endpoint does not exceed n.

In the case of even s.a. differential operations, we are able to make several additional assertions, in particular, to confirm some facts from the previous sections in a simple way. For an even s.a. differential operation, the deficiency indices of the associated initial symmetric operator are always equal, $m_\pm = m$, and we obtain the equality

$$m = \frac{1}{2}\left[p(a) + p(b)\right]. \tag{4.119}$$

We dwell on the interesting case, considered in Sect. 4.4, that one of the endpoints of the interval (a, b), let it be a, is regular, while the second endpoint b is singular. In this case, we have $p(a) = n$, while $p(b) \leq n$ and we obtain the estimate $n/2 \leq m \leq n$ known since (4.48). It also follows from (4.119) that $p(b)/2$ is integral, which implies that in the case of the generic even s.a. differential operation, both $p(a)$ and $p(b)$ are even integers. Moreover, as follows from (4.119), a necessary and sufficient condition for the equality $m = n/2$ is $p(b) = 0$, i.e., the triviality of the boundary form at the singular endpoint. As to the sufficiency, it is the assertion of Lemma 4.16; the necessity is its promised converse. The following remark can also be useful. As follows from representations (4.103) and (4.95), (4.96), the inertia indices of the left boundary form at a regular endpoint a are equal to $n/2$ each, $m_\pm(a) = n/2$. The equalities (4.118) with $m_\pm = m$ together with the equality $p(b) = m_+(b) + m_-(b)$ then show once again that $n/2 \leq m \leq n$ and that $p(b)$ is an even integer. In addition, these equalities show that the inertia indices of the right boundary form at the singular endpoint b are equal, $m_+(b) = m_-(b)$, which implies that for the generic even s.a. differential operation, the inertia indices of each, left and right, boundary form are equal. The last remark is as follows. Let us divide the interval (a, b) into two subintervals (a, c) and (c, b), where c is an arbitrary interior point of (a, b). We examine the restrictions $\check{f}_-$ and $\check{f}_+$ of the initial s.a. differential operation $\check{f}$ to the respective subintervals. The corresponding initial symmetric operators $\hat{f}_-$ and $\hat{f}_+$ have the respective deficiency indices

$$m_\pm^{(-)} = m^{(-)} = 1/2\left[p(a) + p(c)\right], \quad m_\pm^{(+)} = m^{(+)} = 1/2\left[p(c) + p(b)\right].$$

But the point c is certainly a regular endpoint for both subintervals, and therefore, $p(c) = n$. Then (4.119) and the last two equalities result in the relation $m = m^{(-)} + m^{(+)} - n$ between the deficiency indices of the initial symmetric operator

$\hat{f}$ and those of the symmetric operators $\hat{f}_-$ and $\hat{f}_+$, which reproduces the already known relation (4.52).

We see that the consequences of the first conclusion are rather extensive.

The second conclusion is that representation (4.111) of the quadratic asymmetry form Δ_{f+} in terms of the a.b. coefficients $\{c_k\}_1^{p(a)+p(b)}$, as well as representation (4.102) of Δ_{f+} in terms of the expansion coefficients $\{c_k\}_1^{m_+ + m_-}$, allows a complete solution of the problem of constructing s.a. operators in $L^2(a,b)$ associated with the initial s.a. differential operation $\check{f}$ similarly to that in Sects. 3.3 and 3.4 with the same conclusions. These s.a. operators, if they exist, are s.a. restrictions of the operator $\hat{f}^+$ associated with $\check{f}$ and defined on the natural domain $D^*_{\check{f}}(a,b)$ and are specified by (asymptotic) s.a. boundary conditions. We formulate a final result as a theorem that can be considered a version of the main theorem, Theorem 3.4, for ordinary differential operators. When formulating its conditions, we repeat the whole set of conditions and facts given and discussed above, so that the theorem can be read independently of the previous text.[41]

Theorem 4.24. *Let $\check{f}$ be an s.a. differential operation of order n on an interval (a,b). Let $\hat{f}^+$ be the operator associated with $\check{f}$ and defined on the natural domain $D^*_{\check{f}}(a,b)$. Let this domain be assigned a linear space $\mathbb{C}^{p(a)+p(b)}$ of a.b. coefficients that is the space of $(p(a)+p(b))$-columns $\{c_k\}_1^{p(a)+p(b)}$ of dimensionless constants characterizing the (asymptotic) behavior of functions $\psi_*(x)$ belonging to $D^*_{\check{f}}(a,b)$ at the endpoints a and b of the interval and having the following origin and properties. The space $\mathbb{C}^{p(a)+p(b)}$ is a direct sum of two linear spaces $\mathbb{C}^{p(a)}$ and $\mathbb{C}^{p(b)}$, where $\mathbb{C}^{p(a)}$ is the space of $p(a)$-component columns $\{c_k(a)\}_1^{p(a)}$ of left a.b. coefficients and $\mathbb{C}^{p(b)}$ is the space of $p(b)$-component columns $\{c_k(b)\}_1^{p(b)}$ of right a.b. coefficients, so that*

$$c_k = \begin{cases} c_k(a), \ k = 1, \dots, p(a), \\ c_{k-p(a)}(b), \ k = p(a)+1, \dots, p(a)+p(b), \end{cases}$$

or

$$\{c_k\}_1^{p(b)+p(a)} = \begin{pmatrix} \{c_k(a)\}_1^{p(a)} \\ \{c_k(b)\}_1^{p(b)} \end{pmatrix}.$$

For regular endpoints[42] a/b, the respective a.b. coefficients are boundary values of functions and their (quasi)derivatives of order $k = 0, \dots, n-1$, so that

[41] Which is partly done for future reference.

[42] The symbol a/b means a and/or b depending on whether both endpoints a and b are regular or one of the endpoints, a or b, is regular.

$p(a/b) = n$, up to some dimensional factor, its own for each k, rendering the a.b. coefficients dimensionless: $c_k(a/b) \sim \psi^{(k-1)}(a/b)$ or $\psi^{[k-1]}(a/b)$ for even $\check{f}$. For singular endpoints a/b, the a.b. coefficients are the coefficients of asymptotic expansions

$$\psi_*(x) = \sum_{k=1}^{p(a/b)} c_k(a/b)\psi_{\mathrm{as}\,k}(a/b, x) + \widetilde{\psi}_{\mathrm{as}}(a/b, x), \ x \to a/b \tag{4.120}$$

(see (4.107) and (4.109)), where $\psi_{\mathrm{as}\,k}(a/b, x)$, $k = 1, \ldots, p(a/b) \leq n$, are linearly independent functions that give finite nonzero contributions to the respective boundary forms $[\psi_*, \psi_*](a/b)$, while $\widetilde{\psi}_{\mathrm{as}}(a/b, x)$ give no contribution; for even $\check{f}$, $p(a/b)$ are even integers. The (quasi)derivatives of functions $\psi_*(x)$ of order up to $n-1$ as $x \to a/b$ are given by directly differentiating asymptotic representations (4.120). In any case, the boundary forms allow the representations, see (4.105), (4.108), (4.106) and (4.110),

$$[\psi_*, \psi_*](a/b) = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(a/b)} \overline{c_k(a/b)}\omega_{kl}(a/b)c_l(a/b),$$

as quadratic forms in the dimensionless a.b. coefficients $c_k(a/b)$ with dimensionless $(p(a/b) \times p(a/b))$ Hermitian matrices $\omega(a/b) = \|\omega_{kl}(a/b)\|$; κ is a factor of dimension of $\check{f}$. The quadratic asymmetry form Δ_{f+} is then represented as a quadratic form in the a.b. coefficients c_k, see (4.111) and (4.112),

$$\Delta_{f+}(\psi_*) = [\psi_*, \psi_*](b) - [\psi_*, \psi_*](a) = 2\mathrm{i}\kappa \sum_{k,l=1}^{p(a)+p(b)} \overline{c_k}\omega_{kl}c_l, \tag{4.121}$$

where the dimensionless $(p(a) + p(b)) \times (p(a) + p(b))$ Hermitian matrix $\omega = \|\omega_{kl}\|$ is block-diagonal[43]

$$\omega = \mathrm{diag}\,(-\omega(a), \omega(b)). \tag{4.122}$$

The Hermitian form $(2\mathrm{i}\kappa)^{-1}\Delta_{f+}$, or the matrix ω, can be reduced to a canonical diagonal form (a reduction to principal axes of inertia) by invertible linear transformations of the a.b. coefficients. This reduction can be done by separately reducing the Hermitian boundary forms $(2\mathrm{i}\kappa)^{-1}[\psi_*, \psi_*](a/b)$, see (4.113) and (4.114),

[43]In some cases, the a.b. coefficients arise as numbers of the same nonzero dimension, in which case the factor $2\mathrm{i}\kappa$ changes to a pure imaginary factor of appropriate dimension, while the matrix ω remains dimensionless.

$$[\psi_*, \psi_*](a/b) = 2\mathrm{i}\kappa \left(\sum_{k=1}^{m_+(a/b)} |c_{+\,k}(a/b)|^2 - \sum_{k=1}^{m_-(a/b)} |c_{-\,k}(a/b)|^2 \right),$$

where the diagonal a.b. coefficients $\{c_{\pm\,k}(a/b)\}_1^{m_\pm(a/b)}$ *are certain linear combinations of the respective a.b. coefficients* $\{c_k(a/b)\}_1^{p(a/b)}$. *The integers* $m_\pm(a/b)$ *are the inertia indices of the respective forms*

$$(2\mathrm{i}\kappa)^{-1}\,[\psi_*, \psi_*]\,(a/b)\,,\ m_+(a/b) + m_-(a/b) = p(a/b).$$

If $\check{f}$ *is even, then the inertia indices are equal, so that we have* $m_+(a/b) = m_-(a/b) = n/2$ *for regular endpoints* a/b *and* $m_+(a/b) = m_-(a/b) = p(a/b)/2$ *for singular endpoints* a/b. *The quadratic asymmetry form is then represented as, see (4.115),*

$$\Delta_{f^+}(\psi_*) = 2\mathrm{i}\kappa \left(\sum_{k=1}^{m_+} |c_{+\,k}|^2 - \sum_{l=1}^{m_-} |c_{-\,k}|^2 \right), \tag{4.123}$$

where the diagonal a.b. coefficients $\{c_{\pm\,k}\}_1^{m_\pm}$,

$$m_+ = m_+(b) + m_-(a),\ m_- = m_-(b) + m_+(a),$$

are given by

$$c_{\pm\,k} = \begin{cases} c_{\pm\,k},\ k = 1, \ldots, m_\pm(b), \\ c_{\mp\,k-m_\pm(b)},\ k = m_\pm(b) + 1, \ldots, m_\pm, \end{cases}$$

or

$$\{c_{\pm\,k}\}_1^{m_\pm} = \left(\{c_{\pm\,k}\}_1^{m_\pm(b)} \big/ \{c_{\mp\,k}\}_1^{m_\mp(a)} \right),$$

where the inertia indices m_+ *and* m_- *of the Hermitian form* $(2\mathrm{i}\kappa)^{-1}\,\Delta_{f^+}$ *are the deficiency indices of the initial symmetric operator* $\hat{f}$ *associated with* $\check{f}$, $\overline{\hat{f}} = \left(f^+\right)^+$; *for even* $\check{f}$ *these indices coincide,* $m_+ = m_-$.

Under the above conditions, the following assertions concerning s.a. differential operators associated with a given s.a. differential operation $\check{f}$ *hold:*

(i) If the inertia indices are different, $m_+ \neq m_-$, *which is possible only for odd or mixed s.a. differential operations, there exists no s.a. differential operator associated with* $\check{f}$.

(ii) If the inertia indices are zero, $m_\pm = 0$, *which implies that all the a.b. coefficients are zero and the quadratic asymmetry form* Δ_{f^+} *is trivial, which*

is possible only if both endpoints, a and b, are singular, then a unique s.a. differential operator associated with $\check{f}$ *is the operator* $\hat{f}^+$.

(iii) If the inertia indices are equal and nonzero, $m_\pm = m > 0$*, then there exists an* m^2*-parameter* $U(m)$ *family* $\{\hat{f}_U, U \in U(m)\}$ *of s.a. operators, associated with* $\check{f}$*. Any s.a. operator* $\hat{f}_U$ *is a restriction of the operator* $\hat{f}^+$ *and is specified by (asymptotic) s.a. boundary conditions defined by an* $m \times m$ *unitary matrix* $U = \|U_{kl}\|$ *establishing the isometric relation*

$$\{c_{-k}\}_1^m = U\{c_{+k}\}_1^m, \tag{4.124}$$

or

$$c_{-k} = \sum_{k=1}^{m} U_{kl} c_{+l}, \tag{4.125}$$

between the diagonal a.b. coefficients $\{c_{-\,k}\}_1^m$ *and* $\{c_{+\,k}\}_1^m$*. Conversely, an isometric relation (4.124), or (4.125), between the diagonal a.b. coefficients with an arbitrary* $m \times m$ *unitary matrix* U *defines an s.a. operator associated with* $\check{f}$.

In other words, the domain D_{f_U} of an s.a. operator $\hat{f}_U$ associated with $\check{f}$ is a subspace of functions $\psi_*(x)$ belonging to the natural domain $D^*_{\check{f}}(a,b)$ and additionally satisfying (asymptotic) s.a. boundary conditions defined by (4.124), or (4.125). If $\check{f}$ is regular, i.e., both endpoints of the interval are regular, then the s.a. boundary conditions can be given a conventional form of a finite relation between the boundary values of functions and their (quasi)derivatives of order up to $n-1$ at the endpoints—this relation is determined by relation (4.124), or (4.125)—and a linear relation connecting these boundary values with the diagonal a.b. coefficients. If at least one of the endpoints a/b is singular and the associated a.b. coefficients are not identically zero (the corresponding boundary form $[\psi_*, \psi_*](a/b)$ is nontrivial), then the corresponding asymptotic s.a. boundary conditions are given by asymptotic expansions (4.120), by a linear relation connecting the a.b. coefficients, including the boundary values of functions and their (quasi)derivatives of order up to $n-1$ at a regular endpoint if it exists, and the diagonal a.b. coefficients, and by relation (4.124), or (4.125), between the diagonal a.b. coefficients.

In the case of even s.a. differential operations where $m_+(a/b) = m_-(a/b) = p(a/b)/2$, the matrix U can be of a block-diagonal form

$$U = \operatorname{diag}(U(b), U(a)), \tag{4.126}$$

where the $p(a)/2 \times p(a)/2$ unitary matrix $U(a)$ establish an isometric relation between the left diagonal a.b. coefficients $c_{-\,k}(a)$ and $c_{+\,k}(a)$ (associated with the left endpoint a), while $p(b)/2 \times p(b)/2$ unitary matrix $U(b)$ establish an isometric relation between the right diagonal a.b. coefficients $c_{+\,k}(b)$ and $c_{-\,k}(b)$ (associated with the right endpoint b). We call the (asymptotic) s.a. boundary conditions defined by a unitary matrix U of block-diagonal form (4.126) the *split s.a. boundary* *conditions*, they are divided into two separate independent sets of (asymptotic) boundary conditions for each endpoint of the interval, see also Sect. 4.6.

As an illustration, we consider an application of the asymmetry form method to regular even s.a. differential operations. This method allows us to solve completely and simply the problem of constructing s.a. differential operators associated with such operations.

Let $\check{f}$ be a regular even s.a. differential operation of order n on a finite interval $[a,b]$. A reduction of representation (4.97) for the sesquilinear asymmetry form ω_{f+} in this case to the diagonal $\chi_* = \psi_*$ yields the following representation for the quadratic asymmetry form[44]:

$$\Delta_{f+}(\psi_*) = \Psi_*^+(b)\,\mathcal{E}\Psi_*(b) - \Psi_*^+(a)\,\mathcal{E}\Psi_*(a)\,, \tag{4.127}$$

where the $n \times n$ matrix $\mathcal{E}$ is given by (4.66), while the n-columns $\Psi_*(a)$ and $\Psi_*(b)$ are given by (4.68) with the change of subscript $U \to *$,

$$\Psi_{*k}(a) = \psi_*^{[k-1]}(a)\,,\ \Psi_{*k}(b) = \psi_*^{[k-1]}(b)\,, k = 1,\ldots,n.$$

We now make an important preliminary remark related to dimensional considerations. In the mathematical literature, the variable x and functions ψ_* are considered dimensionless, so that the quantities $\psi_*, \psi_*^{[1]}, \ldots, \psi_*^{[n-1]}$ are of the same zero dimension, as well as the differential operation $\check{f}$ itself. Therefore, when comparing representation (4.127) with representation (4.121) and (4.122), where $p(a) + p(b) = 2n$ and $\kappa = 1$, as is conventionally adopted in the mathematical literature, we could immediately identify the a.b. coefficients $\{c_k\}_1^{2n}$ with the corresponding boundary values,

$$\{c_k\}_1^{2n} = \left(\left\{\psi_*^{[k-1]}(a)\right\}_1^n \Big/ \left\{\psi_*^{[k-1]}(b)\right\}_1^n\right),$$

and the $2n \times 2n$ Hermitian matrix ω would be $\omega = (1/2i)\,\mathrm{diag}\,(-\mathcal{E},\mathcal{E})$. But in physics, the variable x is assigned a certain dimension, the dimension of length, which we write as $[x] = [\text{length}]$, whereas $[\psi_*] = [\text{length}]^{-1/2}$. If we assume that the first coefficient function $f_n(x)$ of $\check{f}$ is dimensionless,[45] then $[\psi_*^{[k]}] = [\text{length}]^{-k-1/2}$, $[\check{f}] = [\text{length}]^{-n}$, and $[\Delta_{f+}] = [\text{length}]^{-n}$.

According to our convention, the left and right a.b. coefficients $c_k(a/b)$ coincide with the respective boundary values $\psi_*^{[k-1]}(a/b)$ up to a dimensional factor, specific for each k, so that all the a.b. coefficients are dimensionless, or are of the same dimension, and the matrix ω is dimensionless. In our case, this can be accomplished as follows We introduce an arbitrary, but fixed, parameter τ of dimension of length,

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[44]We could equivalently use representation (4.103) for the quadratic boundary form at a regular endpoint.

[45]Which can always be done by multiplying $\check{f}$ by an appropriate inessential constant dimensional factor.

$[\tau] = $ [length] (in particular, we can take the length $l = b - a$ of the interval for such a parameter), and define the n-columns of left and right a.b. coefficients by

$$\{c_k(a/b)\}_1^n = \{\Psi_{\tau\,k}\,(a/b)\}_1^n = \Psi_\tau(a/b),\ \Psi_{\tau\,k}\,(a/b) = \tau^{k-1}\psi_*^{[k-1]}\,(a/b)\,.$$

All the a.b. coefficients are of dimension $[\text{length}]^{-1/2}$. In terms of these a.b. coefficients $\Psi_{\tau\,k}(a/b)$, the asymmetry form Δ_{f+} is represented as

$$\Delta_{f+}\,(\psi_*) = \tau^{-n+1}\left[\Psi_\tau^+\,(b)\,\mathcal{E}\Psi_\tau\,(b) - \Psi_\tau^+\,(a)\,\mathcal{E}\Psi_\tau\,(a)\right],$$

and the matrix ω is the same. We can now proceed to reducing the Hermitian form $-i\tau^{n-1}\Delta_{f+}\,(\psi_*)$ to a canonical diagonal form. We separately reduce the left and right Hermitian quadratic boundary forms $-i\Psi_\tau^+\,(a)\,\mathcal{E}\Psi_\tau\,(a)$ and $-i\Psi_\tau^+\,(b)\,\mathcal{E}\Psi_\tau\,(b)$ to a canonical diagonal form, which is equivalent to diagonalizing the matrix $-i\mathcal{E}$. But the latter has already been done; see (4.95) and (4.96). The final representation for Δ_{f+} is

$$\Delta_{f+}\,(\psi_*) = i\tau^{-n+1}\left[\Psi_{\tau+}^+\Psi_{\tau+} - \Psi_{\tau-}^+\Psi_{\tau-}\right], \tag{4.128}$$

where the n-component columns $\Psi_{\tau+}$ and $\Psi_{\tau-}$ of the diagonal a.b. coefficients are given by

$$\Psi_{\tau+} = \left(\Psi_{\tau+}\,(b)\,\big/\,\Psi_{\tau-}\,(a)\right),\ \Psi_{\tau-} = \left(\Psi_{\tau-}\,(b)\,\big/\,\Psi_{\tau+}\,(a)\right), \tag{4.129}$$

where in turn $\Psi_{\tau\pm}\,(a/b)$ are the $n/2$-component columns with the components $\Psi_{\tau\pm,k}\,(a/b)$, $k = 1,\ldots,n/2$, given by

$$\Psi_{\tau+,k}\,(a/b) = \sqrt{\frac{1}{2}}\left[\tau^{k-1}\psi_*^{[k-1]}\,(a/b) + i\tau^{n-k}\psi_*^{[n-k]}\,(a/b)\right], \tag{4.130}$$

$$\Psi_{\tau-,k}\,(a/b) = \sqrt{\frac{1}{2}}\left[\tau^{n/2-k}\psi_*^{[n/2-k]}\,(a/b) - i\tau^{n/2+k-1}\psi_*^{[n/2+k-1]}\,(a/b)\right]. \tag{4.131}$$

According to Theorem 4.24, it follows from representation (4.128) that the s.a. boundary conditions specifying an s.a. operator $\hat{f}_U$ are given by

$$\Psi_{U,\tau-} = U\Psi_{U,\tau+}, \tag{4.132}$$

where U is an $n\times n$ unitary matrix and the columns $\Psi_{U,\tau\pm}$ differ from the general columns $\Psi_{\tau\pm}$ (4.129)–(4.131) by the change $*\to U$ of the index at the functions indicating the belonging of the corresponding functions to the domain D_{f_U} of $\hat{f}_U$. As U ranges over all the group $U\,(n)$, we obtain the whole n^2-parameter $U\,(n)$ family $\{\hat{f}_U,\ U \in U\,(n)\}$ of s.a. differential operators associated with the given regular even s.a. differential operation $\check{f}$ of order n.

We complete this item with several obvious remarks.

Remark 4.25. (1) We used the same symbol $\hat{f}_U$ to denote s.a. operators associated with $\check{f}$ as in Sect. 4.6, although the subscript U here has a somewhat different meaning. In the previous context, the subscript U was the symbol of an s.a. extension of an initial symmetric operator $\hat{f}$ generated by an isometry $\hat{U} : D_+ \longmapsto D_-$ of its deficient subspaces. In the present context, this is the symbol of an s.a. restriction of the adjoint operator $\hat{f}^+ = \hat{f}^*$ generated by the isometric mapping (4.132) of one set of diagonal a.b. coefficients to another one.

(2) We could organize the column $\Psi_{\tau -}$ in a different way, for example, as follows:

$$\Psi_{\tau -} \to \Xi \Psi_{\tau -} = (\Psi_{\tau +}(a) \diagup \Psi_{\tau -}(b)),$$

where $\Xi = \text{antidiag}\,(I, I)$ is an $n \times n$ unitary matrix, I is the $n/2 \times n/2$ identity matrix. Then the unitary matrix U in (4.132) would change to the matrix ΞU, which is also unitary.

(3) It is evident that we can define s.a. boundary conditions by the relation $\Psi_{\tau +} = U\Psi_{\tau -}$. To this end, it is sufficient to make the replacement $U \to U^{-1}$ in (4.132).

(4) If the matrix U in (4.132) is of block-diagonal form (7.6), $U = \text{diag}\,(\,U\,(b)\,, U\,(a)\,)$, where $U\,(a)$ and $U\,(b)$ are $n/2 \times n/2$ unitary matrices, we obtain the split s.a. boundary conditions

$$\Psi_{\tau +}(a) = U\,(a)\,\Psi_{\tau -}(a)\,,\ \Psi_{\tau -}(b) = U\,(b)\,\Psi_{\tau +}(b)\,.$$

The asymmetry form method also works well as applied to singular even s.a. differential operations $\check{f}$ in the case that one endpoint of the interval, let it be the left endpoint a, is regular, while the second one, the right endpoint b, is singular and the right boundary form is trivial, $[\psi_*, \psi_*]\,(b) = 0$. In this case, the asymmetry form Δ_{f+} allows the representation following from (4.128) with $\Psi_{\tau \pm}(b) = 0$:

$$\Delta_{f+}(\psi_*) = i\,\tau^{-n+1}\left[\Psi^+_{\tau -}(a)\,\Psi_{\tau -}(a) - \Psi^+_{\tau +}(a)\,\Psi_{\tau +}(a)\right], \tag{4.133}$$

where the $n/2$-component columns $\Psi_{\tau \pm}(a)$ of the left diagonal a.b. coefficients are given by (4.130) and (4.131). It follows from representation (4.133) that the s.a. boundary conditions specifying an s.a. operator $\hat{f}_U$ associated with $\check{f}$ are given by

$$\Psi_{U,\tau +}(a) = U\Psi_{U,\tau -}(a)\,, \tag{4.134}$$

where U is a unitary $n/2 \times n/2$ unitary matrix and the columns $\Psi_{U,\tau \pm}(a)$ differ from the general columns $\Psi_{\tau \pm}(a)$ (4.130) and (4.131) by the change $* \to U$ of the index at the functions indicating the belonging of the corresponding functions to the domain D_{f_U} of $\hat{f}_U$. As U ranges over all the group $U\,(n/2)$, we obtain the whole

$(n/2)^2$-parameter $U(n/2)$ family $\{\hat{f}_U,\ U \in U(n/2)\}$ of s.a. differential operators associated with the given singular even s.a. differential operation $\check{f}$ of order n.

Of course, we can interchange the columns $\Psi_{\tau -}(a)$ and $\Psi_{\tau +}(a)$ in (4.134), as well as repeat a remark similar to Remark 4.25 following (4.132) and concerning the new meaning of the symbol $\hat{f}_U$. We also note that representation (4.133) manifestly confirms the above assertion about the deficiency indices of the initial symmetric operator $\hat{f}$ associated with a singular s.a. differential operation $\check{f}$ of order n in the case that one endpoint of the interval is regular while another endpoint is singular: for $\hat{f}$ to have the minimum possible deficiency indices $(n/2, n/2)$, it is necessary and sufficient that the boundary form at the singular endpoint be trivial.

In conclusion, we note that the specification of s.a. differential operators associated with such s.a. differential operations by s.a. boundary conditions (4.134) is in complete agreement with the previous specification according to Theorems 4.17 and 4.22. We only repeat that the application of Theorem 4.17 requires an explicit evaluation of the deficient subspaces and that the matrix $A_{1/2}$ in Theorem 4.22 is defined up to the change $A_{1/2} \to A_{1/2}Z$, where Z is a nonsingular matrix, while s.a. boundary conditions (4.134) do not require evaluating the deficient subspaces and contain no arbitrariness.

Chapter 5
Spectral Analysis of Self-adjoint Operators

5.1 Preliminaries

Constructing an s.a. operator for a given physical quantity is only the first part of the QM problem associated with this quantity. The second part is solving the spectral problem, i.e., a spectral analysis of the obtained observable. In this book, we mainly deal with s.a. differential operators, at least in what concerns physical applications. In spectral analysis of operators, we restrict ourselves to finding their spectra and deriving formulas for (generalized) eigenfunction expansions; following[1] [9, 116], we call the latter the *inversion formulas*. These formulas are a foundation for a physical probabilistic interpretation of measuring the observable.

Before going into mathematical details, we outline a treatment of spectral analysis conventional for physics literature, or a physical approach to the spectral problem; in passing, we briefly recall basic notions concerning the spectrum of an s.a. operator; see Chap. 2.

Standard textbooks on QM for physicists treat the spectral problem as the eigenvalue problem similarly to the finite-dimensional case. We recall that a number $\lambda \in \mathbb{C}$ and a vector $\xi_\lambda \in D_f$ are respectively called an eigenvalue of the operator $\hat{f}$ and an eigenvector of $\hat{f}$ corresponding to the eigenvalue λ if

$$\hat{f}(\lambda)\,\xi_\lambda = 0,\ \hat{f}(\lambda) = \hat{f} - \lambda\hat{I} = \hat{f} - \lambda\hat{I}_{D_f}, \tag{5.1}$$

or $\xi_\lambda \in \ker\hat{f}(\lambda)$, the eigenspace of $\hat{f}$ corresponding to the eigenvalue λ; see Sect. 2.3.1. In the finite-dimensional case, the spectrum spec $\hat{f}$ of an operator $\hat{f}$ is defined as the set of all its eigenvalues, spec $\hat{f} = \{\lambda : \ker\hat{f}(\lambda) \neq \{0\}\}$. The operator $\hat{\mathcal{R}}(z) = (\hat{f}(z))^{-1}$ does not exist for $z \in$ spec $\hat{f}$, whereas for all other z,

[1]There exist recent monographs on spectral theory for unbounded self-adjoint operators and its application to QM; see for example [43, 92, 95, 145].

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$z \notin \operatorname{spec} \hat{f}$, it exists and is bounded. In the n-dimensional Euclidian space with a fixed basis, an s.a. operator is defined by a Hermitian $n \times n$ matrix. Its spectrum is real, and the eigenvectors of the matrix form an orthogonal basis in this space.

As was already said in Sect. 2.5, in the case of an infinite-dimensional Hilbert space $\mathfrak{H}$, there exists another, third, possibility for the operator $\hat{\mathcal{R}}(z)$ at some z: it exists, but is unbounded or is bounded, but is not densely defined. The corresponding z are also assigned to the spectrum of $\hat{f}$.

In the infinite-dimensional case, the definition of the spectrum of an operator $\hat{f}$, similarly to the finite-dimensional case, as the set of eigenvalues is not suitable. Indeed, by definition (5.1), all the eigenvectors must belong to the Hilbert space, $\xi_\lambda \in \mathfrak{H}$, $\forall \lambda$. But with this definition of spectrum, we can miss a part of the spectrum's points, in which case the admissible eigenvectors ξ_λ do not form a complete set of vectors in $\mathfrak{H}$, and we cannot afford the probabilistic interpretation of QM. That is why in the physical approach, the condition $\xi_\lambda \in \mathfrak{H}$ is not imposed from the beginning. For differential operators, the spectral problem is treated as the conventional eigenvalue problem for differential equations, ordinary or partial. Eigenvalues enter such equations as numerical parameters.

The first question for a physicist to be solved is which values of the parameters can be considered the spectrum points of the corresponding differential operator. If we do not require that $\xi_\lambda \in \mathfrak{H}$, there are no restrictions on these parameters from a formal mathematical standpoint. But physicists effectively use heuristic, physical, considerations that restrict admissible values of these parameters. Among these are appropriate boundary conditions, the requirement for eigenfunctions to be locally square-integrable, the requirement for eigenfunctions of bound states to vanish at spatial infinity so that their norms will be finite; an eigenfunction may not vanish at infinity, but become a plane wave corresponding to a free motion of particles. Such functions are "normalized to δ-function," and so on. In many cases, such physical considerations allow finding both the discrete eigenvalues for bound states and the continuous part of the spectrum for unbound states. But then the question arises whether the obtained eigenfunctions form a complete set in $\mathfrak{H}$.

In solving this problem in the case of a pure discrete spectrum, physicists use the well-studied properties of special functions and the well-developed general theory of Fourier series expansions with respect to special functions. In the presence of a continuous spectrum, the situation is more complicated. No regular methods for proving the completeness of eigenfunctions including the eigenfunctions of the continuous spectrum, even if they are orthonormalized to a delta function, are known. It is safe to say that in many cases, the construction of a complete set of eigenfunctions and especially a proof of its completeness seem to be an art. All this suggests that the formulation of the spectral problem in the infinite-dimensional case has to be modified in comparison with the finite-dimensional case. A proper formulation of the spectral problem for s.a. operators and its general solution are well known in the mathematical literature under the name of spectral analysis. For s.a. ordinary differential operators, we now have different well-elaborated methods for finding the spectrum and constructing the corresponding (generalized) eigenfunction expansions. The probabilistic interpretation of QM is formulated in terms of spectral resolutions of s.a. operators.

We begin by recalling necessary notions and facts concerning the spectrum of an s.a. operator $\hat{f}$ in an infinite-dimensional Hilbert space; see Sects. 2.5 and 2.8.6.

A number $z \in \mathbb{C}$ is called a regular point, or a point of the resolvent set (regp $\hat{f}$), of an operator $\hat{f}$ if the operator $\hat{\mathcal{R}}(z) = \hat{f}(z)^{-1} = (\hat{f} - z\hat{I})^{-1}$ exists and is bounded and defined everywhere. In this case, the operator $\hat{\mathcal{R}}(z)$ is called the resolvent of the operator $\hat{f}$. For a regular point z, the equation $\hat{f}(z)\xi = \eta$ with any $\eta \in \mathfrak{H}$ is uniquely resolvable with respect to ξ: $\xi = \hat{\mathcal{R}}(z)\eta$. The complement of the resolvent set regp$\hat{f}$ to the whole complex plane $\mathbb{C}$ is called the spectrum of the operator $\hat{f}$ and is denoted by spec $\hat{f}$. The points of the spectrum are usually denoted by λ, or by E if $\hat{f}$ is a Hamiltonian. The resolvent set of an s.a. operator is an open set, and any complex $z \in \mathbb{C}'$ (Im $z \neq 0$), is a regular point; it follows that the spectrum of an s.a. operator is a closed real set. It is evident that the eigenvalues of the operator $\hat{f}$ belong to its spectrum; they form the so-called point spectrum.

If λ belongs to the point spectrum, the operator $\hat{f}(\lambda)$ is noninvertible. The point spectrum of an s.a. operator in a separable Hilbert space (we recall that we restrict ourselves to such spaces) is at most countable.

The union of the closure of the point spectrum in the whole spectrum and the eigenvalues of infinity multiplicity forms the continuous spectra. It may be that the intersection of the point and continuous spectra is not empty: a spectrum point λ may belong to the point spectrum and to the continuous spectrum simultaneously.

A real number λ is in spec $\hat{f}$ if either (a) the operator $\hat{\mathcal{R}}(\lambda)$ does not exist, in which case λ is an eigenvalue of $\hat{f}$, or (b) the operator $\hat{\mathcal{R}}(\lambda)$ exists but is unbounded.

In what follows, we present the basic notions of the general spectral theory of s.a. operators and its application to the spectral analysis of s.a. ordinary differential operators. Our exposition is organized as a set of definitions and statements (theorems) and closely follows that of [9, 116], except that proofs are abandoned. The subsequent chapters contain a number of illustrations of the general theory.

We note that in all the known examples considered on the basis of physical arguments, the results are confirmed by the rigorous approach. Nevertheless, even in these cases, the advantage of the rigorous approach is justified by the fact that in this approach, the necessity of applying physical considerations (being, in essence, an art) is replaced by a set of mathematically well formulated rules.

5.2 Spectral Decomposition of Self-adjoint Operators

5.2.1 Identity Resolution

The notion of identity resolution is formulated in terms of orthoprojectors; see Chap. 2.

Definition 5.1. A family of orthoprojection operators $P(\lambda)$ defined on the real axis, $\lambda \in \mathbb{R}$, is called an *identity resolution* (IRin what follows)[2] if it has the following properties:

(a) $P(\lambda) \leq P(\mu)$ for $\lambda < \mu$ (which is equivalent to $P(\lambda)P(\mu) = P(\mu)P(\lambda) = P(\lambda)$ for $\lambda < \mu$)
(b) $P(\lambda + 0) = P(\lambda)$
(c) $P(-\infty) = 0$, $P(+\infty) = \hat{I}$

(the equalities (b) and (c) are meant in the strong sense).

Theorem 5.2. *Any s.a. operator $\hat{f}$ with domain D_f uniquely defines an IR such that:*

(a) A vector ξ belongs to D_f iff

$$\int_{-\infty}^{\infty} \lambda^2 \mathrm{d}\|P(\lambda)\xi\|^2 < \infty.$$

(b) The operator $\hat{f}$ has the following integral representation:

$$\hat{f}\xi = \int_{-\infty}^{\infty} \lambda \mathrm{d}P(\lambda)\xi, \quad \forall \xi \in D_f, \tag{5.2}$$

which implies that

$$\|\hat{f}\xi\|^2 = \int_{-\infty}^{\infty} \lambda^2 \mathrm{d}\|P(\lambda)\xi\|^2 < \infty.$$

Integrals in (5.2) are operator analogues of the Lebesgue–Stieltjes integrals; see [9, 116].

Conversely, any operator $\hat{f}$ that is defined by (5.2) with a certain IR $P(\lambda)$ on the domain D_f of item (a) is s.a., and its IR coincides with $P(\lambda)$.

In addition, a bounded operator $\hat{S}$ defined on the whole Hilbert space $\mathfrak{H}$ commutes with $\hat{f}$ iff it commutes with $P(\lambda)$ for any λ.

[2] Another name is "an (operator) spectral function."

We call λ_0 the *constancy point of an IR* $P(\lambda)$ if there exists a neighborhood U_{λ_0} of λ_0 where $P(\lambda)$ is constant. An open set (see item (a) in Theorem 5.3 below) of all constancy points of $P(\lambda)$ is denoted by Cn_P. The closed set Gr_P that is the complement of Cn_P in $\mathbb{R}$ is called the *growth set of* $P(\lambda)$. A point λ is called the *jump point* of $P(\lambda)$ if the orthoprojector $\Pi_\lambda \equiv P(\lambda) - P(\lambda - 0)$ is not zero.

Theorem 5.3. *Let $P(\lambda)$ be the IR of an s.a. operator $\hat{f}$. Then the following assertions hold.*

(a) A real number λ is a regular point of $\hat{f}$ iff $\lambda \in Cn_P$ (which implies that Cn_P is a open set).
(b) The spectrum of $\hat{f}$ coincides with Gr_P, the growth set of $P(\lambda)$.
(c) A real number λ is an eigenvalue of $\hat{f}$ iff λ is a jump point of $P(\lambda)$, $\Pi_\lambda \neq 0$; Π_λ is the projection operator on the corresponding eigenspace of $\hat{f}$.

5.2.2 *Degeneracy of the Spectrum*

In the finite-dimensional case, in which the spectrum of an operator coincides with the set of its eigenvalues, the spectrum is called simple if the multiplicity of each eigenvalue is one. Otherwise, the spectrum is said to be degenerate. For operators in infinite-dimensional Hilbert spaces, the spectrum generally does not coincide with the set of eigenvalues, and such a definition becomes unsuitable. In what follows, we discuss a general definition of degeneracy, in particular, simplicity, of a spectrum for s.a. operators in Hilbert spaces.

We first introduce the notion of generating vector for an s.a. operator $\hat{f}$ with the IR $P(\lambda)$ and a definition of s.a. operator with a *simple spectrum*.

Definition 5.4. A vector $\xi_g \in \mathfrak{H}$ is called a generating vector[3] of an s.a. operator $\hat{f}$ if the linear envelope of vectors $\xi_g(\Delta) = \Pi(\Delta)\xi_g$ is dense in $\mathfrak{H}$.

Here, Δ denotes an arbitrary interval of the real axis. If the interval is closed, $\Delta = [\lambda_1, \lambda_2]$, $\lambda_1 \leq \lambda_2$, then $\Pi(\Delta)$ is defined by $\Pi(\Delta) = P(\lambda_2) - P(\lambda_1 - 0)$, and if $\Delta = (\lambda_1, \lambda_2]$, then $\Pi(\Delta) = P(\lambda_2) - P(\lambda_1)$, and similarly for intervals of other types.

Definition 5.5. A spectrum of an s.a. operator $\hat{f}$ is called simple[4] if the operator has a generating vector.

If the spectrum is simple, its point spectrum (if it exists) is nondegenerate.

It is useful to introduce the notion of the Hilbert space L^2_σ of functions $\varphi(\lambda)$, $\lambda \in \mathbb{R}$, which is defined as follows. We call any real nondecreasing function $\sigma(\lambda)$

[3]Another name is "cyclic vector."

[4]Nondegenerate in physics terminology.

continuous from the right a *spectral function*. Let a spectral function be given. To avoid the trivial case, we assume that $\sigma(\lambda)$ is nonconstant. Then by analogy with the Lebesgue measure, we can introduce the notion of a σ-measurable set defining a σ-measure $\tilde{\sigma}(\Delta)$ of intervals by

$$\tilde{\sigma}(\Delta) = \sigma(\lambda_2) - \sigma(\lambda_1 - 0),\ \Delta = [\lambda_1, \lambda_2],\ \ \lambda_1 \leq \lambda_2,$$

and similarly for intervals of other types.

The σ-measure of a nonzero interval is zero if the interval is a constancy interval of the spectral function, while $\tilde{\sigma}([\lambda, \lambda]) = \sigma(\lambda) - \sigma(\lambda - 0)$ differs from zero if λ is a discontinuity point of $\sigma(\lambda)$. Using a σ-measure, we can define σ-measurable functions and the Lebesgue–Stieltjes integral $\int \varphi(\lambda)\mathrm{d}\sigma(\lambda)$. The Hilbert space L^2_σ is defined as the linear space of σ-measurable functions of finite σ-norm $\int |\varphi(\lambda)|^2 \mathrm{d}\sigma(\lambda)$ with the scalar product

$$(\varphi_1, \varphi_2) = \int \overline{\varphi_1(\lambda)}\varphi_2(\lambda)\mathrm{d}\sigma(\lambda),\ \varphi_1, \varphi_2 \in L^2_\sigma.$$

Details of the construction can be found in [9, 116, 141].

Let Λ_σ denote the operator in L^2_σ defined as

$$\Lambda_\sigma : \begin{cases} D_\Lambda = \left\{\varphi : \varphi(\lambda), \lambda\varphi(\lambda) \in L^2_\sigma\right\}, \\ \Lambda_\sigma\varphi(\lambda) = \lambda\varphi(\lambda). \end{cases}$$

This operator is called the operator of multiplying by independent variable. The following assertions hold:

(a) The operator Λ_σ is s.a.
(b) The spectrum of Λ_σ is simple, and any function $\varphi(\lambda) \in L^2_\sigma$ different from zero at any point λ is a generating vector of Λ_σ.

It is useful to introduce the so-called improper generating element of an s.a. operator $\hat{f}$.

Definition 5.6. An arbitrary vector function $\xi_g(\Delta)$ of intervals $\Delta \in R$ that takes values in the Hilbert space $\mathfrak{H}$ is called an improper generating element of an s.a. operator $\hat{f}$ if

(a) $\Pi(\Delta_1)\xi_g(\Delta_2) = \xi_g(\Delta_1)$ for $\Delta_1 \subseteq \Delta_2$ ($\Pi(\Delta)$ is constructed with respect to IR $P(\lambda)$ of the operator $\hat{f}$).
(b) The linear envelope of vectors $\xi_g(\Delta)$ is dense in $\mathfrak{H}$.

It is evident that if ξ_g is a generating vector of an s.a. operator $\hat{f}$, then $\xi_g(\Delta) = \Pi(\Delta)\xi_g$ is its improper generating element with the property

$$\xi_g = \mathrm{s}\lim_{\lambda_1 \to \infty, \lambda_2 \to -\infty} \xi_g(\Delta),\ \Delta = [\lambda_1, \lambda_2].$$

It appears that conversely, if an s.a. operator $\hat{f}$ has an improper generating element $\xi_g(\Delta)$, then this operator also has a generating vector ξ_g, and therefore a simple spectrum (see Theorem 5.7 below); in particular, if the strong limit $\mathrm{s}\lim_{\lambda_1\to\infty,\lambda_2\to-\infty}\xi_g(\Delta)=\xi_g$ exists, then the vector ξ_g is a generating vector, and $\xi_g(\Delta)=\Pi(\Delta)\xi_g$.

Theorem 5.7. *Let an s.a. operator $\hat{f}$ have an improper generating element $\xi_g(\Delta)$. Let a spectral function $\sigma(\lambda)$ and a vector function $\chi(\lambda)\in\mathfrak{H}$ be defined by*

$$
\begin{aligned}
&\sigma(\lambda)=\varepsilon(\lambda)\tilde{\sigma}(\Delta_\lambda),\ \tilde{\sigma}(\Delta_\lambda)=|\xi_g(\Delta_\lambda)|^2,\ \sigma(0)=0,\\
&\chi(\lambda)=\varepsilon(\lambda)\xi_g(\Delta_\lambda),\ \lambda\neq 0,\ \chi(0)=0,\\
&\varepsilon(\lambda)=\operatorname{sgn}\lambda,\ \ \Delta_\lambda=\begin{cases}(0,\lambda],\ \lambda>0,\\ (\lambda,0],\ \lambda<0.\end{cases}
\end{aligned} \tag{5.3}
$$

Then the formulas

$$
\xi=\int_{-\infty}^{+\infty}\varphi(\lambda)\mathrm{d}\chi(\lambda),\ \ \hat{f}\xi=\int_{-\infty}^{+\infty}\lambda\varphi(\lambda)\mathrm{d}\chi(\lambda)
$$

establish an isometric map of L^2_σ onto $\mathfrak{H}$, $L^2_\sigma\longmapsto\mathfrak{H}$ with $\Lambda_\sigma\longmapsto\hat{f}$. If $\varphi_g(\lambda)$ is a generating vector of the operator Λ_σ, then the corresponding vector ξ_g is the generating vector of the operator $\hat{f}$, which implies that $\hat{f}$ has a simple spectrum.

Self-adjoint operators with multiple spectrum are defined similarly.

Definition 5.8. A set of vectors $\xi_{i,g}\in H$, $i=1,\dots,k$, is called a generating basis of an s.a. operator $\hat{f}$ if the linear envelope of vectors $\xi_{i,g}(\Delta)=\Pi(\Delta)\xi_{i,g}$ is dense in $\mathfrak{H}$. The generating basis of a given $\hat{f}$ is not defined uniquely. It is evident that the number k of generating basis vectors is bounded from below and not bounded from above: we always can extend a generating basis by adding a new basis vector.

Definition 5.9. The minimum admissible number m of the generating basis vectors is called the *multiplicity of the spectrum* of $\hat{f}$, and the spectrum is called m-fold. If the multiplicity satisfies $m>1$, the spectrum is called multiple.[5]

In the case of finite-dimensional spaces, the multiplicity of a spectrum thus defined coincides with the maximum degeneracy of eigenvalues.

Just as an s.a. operator with simple spectrum is conveniently represented in terms of the Hilbert spaces L^2_σ, so an s.a. operator with m-fold spectrum is conveniently represented in terms of the Hilbert space $L^2_{m\sigma}$. The latter notion is defined in terms of the so-called matrix spectral function.

[5]In the physics literature, the term "degenerate spectrum" is conventionaly used.

5.2.3 Matrix Spectral Function

Any Hermitian matrix function $\sigma_{ij}(\lambda)$, $\lambda \in \mathbb{R}, i, j = 1, \ldots, k$, nondecreasing (i.e., the matrix $\sigma_{ij}(\lambda) - \sigma_{ij}(\lambda')$ is positive semidefinite for $\lambda > \lambda'$) and continuous from the right is called a *matrix spectral function.* To avoid the trivial case, we assume that $\sigma_{ij}(\lambda)$ is nonconstant. We note that we make no reservations on the rank of the matrix $\sigma_{ij}(\lambda)$; it may be not maximum even at all λ.

A matrix spectral function generates the Hilbert space $L^2_{k\sigma}$ of k-component vector functions $\varphi(\lambda) = \left\{\varphi^i(\lambda),\, i = 1, \ldots k,\, \lambda \in \mathbb{R}\right\}$ with the scalar product given by

$$(\varphi, \varphi') = \int \overline{\varphi^i(\lambda)}\varphi'^j(\lambda) \mathrm{d}\sigma_{ij}(\lambda). \tag{5.4}$$

Elements $\varphi(\lambda)$ of this Hilbert space have finite norms induced by scalar product (5.4). Details can be found in [9, 116, 141].

An example of an s.a. operator with multiple spectrum is the operator Λ_σ of multiplying by the independent variable in $L^2_{k\sigma}$:

$$\Lambda_\sigma : \begin{cases} D_\Lambda = \left\{\varphi : \varphi(\lambda), \lambda\varphi(\lambda) \in L^2_{k\sigma}(a, b)\right\}, \\ \Lambda_\sigma\varphi(\lambda) = \lambda\varphi(\lambda) = \{\lambda\varphi^i(\lambda),\, i = 1, \ldots k\}. \end{cases}$$

The multiplicity[6] of its spectrum is less than or equal to k. As a generating basis, we can take k vectors $\varphi_{i,g}(\lambda)$ such that $\varphi^j_{i,g}(\lambda) = \delta^j_i v_i(\lambda)$, where all the functions $v_i(\lambda)$ differ from zero for any λ.

It is useful to introduce the so-called improper generating basis of an s.a. operator $\hat{f}$.

Definition 5.10. An arbitrary set of vector functions $\xi_{i,g}(\Delta)$ of intervals $\Delta \in \mathbb{R}$ that take values in the Hilbert space $\mathfrak{H}$ is called an improper generating basis of an s.a. operator $\hat{f}$ if

(a) $\Pi(\Delta_1)\xi_{i,g}(\Delta_2) = \xi_{i,g}(\Delta_1)$ for $\Delta_1 \subseteq \Delta_2$.
(b) The linear envelope of vectors $\xi_{i,g}(\Delta)$ is dense in $\mathfrak{H}$.

It is evident that if vectors $\xi_{i,g}$ form a generating basis of an s.a. operator $\hat{f}$, then $\xi_{i,g}(\Delta) = \Pi(\Delta)\xi_{i,g}$ is its improper generating basis with the property

$$\xi_{i,g} = \mathrm{s} \lim_{\lambda_1 \to \infty, \lambda_2 \to -\infty} \xi_{i,g}(\Delta),\ \ \Delta = [\lambda_1, \lambda_2],$$

and conversely, if $\xi_{i,g}(\Delta)$ form an improper generating basis and the strong limit $\mathrm{s}\lim_{\lambda_1 \to \infty, \lambda_2 \to -\infty} \xi_{i,g}(\Delta) = \xi_{i,g},\ \ \Delta = [\lambda_1, \lambda_2],$ exists, then the vectors $\xi_{i,g}$ form a generating basis, and $\xi_{i,g}(\Delta) = \Pi(\Delta)\xi_{i,g}$.

An analogue of Theorem 5.7 holds for an improper generating basis.

---

[6]Which is determined by the rank of the matrix $\sigma_{ij}(\lambda)$.

Theorem 5.11. *Let an s.a. operator* $\hat{f}$ *have an improper generating basis* $\xi_{i,g}(\Delta)$*,* $i = 1, \ldots, k$*. Let a matrix spectral function* $\sigma_{ij}(\lambda)$ *and a set of k vectors* $\{\chi_i(\lambda) \in \mathfrak{H},\ i = 1, \ldots, k\}$ *be defined by*

$$\sigma_{ij}(\lambda) = \varepsilon(\lambda)\tilde{\sigma}_{ij}(\Delta_\lambda),\ \tilde{\sigma}_{ij}(\Delta) = (\xi_{i,g}(\Delta), \xi_{j,g}(\Delta)),\ \sigma_{ij}(0) = 0,$$
$$\chi_i(\lambda) = \varepsilon(\lambda)\xi_{i,g}(\Delta_\lambda),\ \lambda \neq 0,\ \chi_i(0) = 0, \tag{5.5}$$

where $\varepsilon(\lambda)$ *and* Δ_λ *are defined in (5.3). Then the relations*

$$\xi = \int_{-\infty}^{+\infty} \sum_{i=1}^{k} \varphi^i(\lambda) \mathrm{d}\chi_i(\lambda),\ \hat{f}\xi = \int_{-\infty}^{+\infty} \sum_{i=1}^{k} \lambda\varphi^i(\lambda) \mathrm{d}\chi_i(\lambda),$$
$$\xi \in \mathfrak{H},\ \ \varphi(\lambda) = \{\varphi^i(\lambda)\} \in L^2_{k\sigma},$$

establish an isometric map $L^2_{k\sigma}$ *onto* $\mathfrak{H}$ *with* $\Lambda_\sigma \longmapsto \hat{f}$*.*

Let $\varphi(\lambda)_{i,g}$*,* $i = 1, \ldots, k$*, be a generating basis of the operator* Λ_σ *in* $L^2_{k\sigma}$*. Then the corresponding set of vectors* $\xi_{i,g} \in \mathfrak{H}$ *is a generating basis of the operator* $\hat{f}$*.*

It thus turns out that if an s.a. operator $\hat{f}$ has an improper generating basis formed by k vector functions $\xi_{i,g}(\Delta)$, then this operator also has a generating basis formed by k generating vectors, and the multiplicity of the spectrum of the operator $\hat{f}$ is less than or equal to k.

5.3 Self-adjoint Differential Operators

5.3.1 Guiding Functionals

In this section, we consider s.a. ordinary differential operators associated with s.a. differential operations of even order.[7] A spectral theory of such operators is well developed. In particular, an even s.a. differential operator of order n always has an improper generating basis formed by n vector functions, which implies that the multiplicity of its spectrum never exceeds n. There exist different methods for constructing complete (sometimes overcomplete) sets of (generalized) eigenfunctions of such operators and the corresponding eigenfunction expansion formulas [9, 24, 27, 70, 71, 101, 108, 116, 129, 148, 149, 162]. The presented list of references is in no way complete. In this book, we follow the *Krein method of guiding functionals* [101] as presented in [9, 116].

[7] We recall that coefficients of even s.a. differential operations are real-valued.

Definition 5.12. Let $\check{f}$ be an s.a. differential operation of finite even order n defined on an interval (a,b), and let $\hat{f}$ be an s.a. operator associated with $\check{f}$ and with domain D_f. A linear functional $\Phi(\xi;z)$ of the form

$$\Phi(\xi;z) = \int_a^b u(x;z)\xi(x)\mathrm{d}x,\ \xi \in \mathbb{D}, \tag{5.6}$$

where $u(x;z)$ is a solution of the homogeneous equation

$$(\check{f} - z)u(x) = 0, \tag{5.7}$$

and $\xi(x)$ is a function belonging to a domain $\mathbb{D}$ that is dense in $L^2(a,b)$ and such that the integral on the right-hand side of (5.6) exists, is called the guiding functional.

In what follows, we introduce a special fundamental system of solutions of (5.7).

Definition 5.13. A fundamental system $u_i(x;z)$ of solutions of (5.7) satisfying the initial conditions

$$u_i^{[j-1]}(c;z) = \delta_{ij},\ i,j = 1,\dots,n, \tag{5.8}$$

where c is a fixed inner point of the interval (a,b), $a < c < b$, is called a *special fundamental system*. If one of the ends of the interval (a,b) is regular, it can be taken for c.

It is evident that the functions $u_i(x;z)$ are real entire in z at any fixed inner point x.

Using a special fundamental system of solutions, we introduce a set of n guiding functionals $\Phi_i(\xi;z)$,

$$\Phi_i(\xi;z) = \int_a^b u_i(x;z)\xi(x)\mathrm{d}x,\ i = 1,\dots,n,\ \ \xi \in \mathbb{D} = \mathcal{D}(a,b).$$

This set of the guiding functionals satisfies the following properties:

1. All $\Phi_i(\xi;z)$ are entire in z for every $\xi \in \mathcal{D}(a,b)$.
2. If $\Phi_i(\xi_0;\lambda_0) = 0$, $i = 1,\dots,n$, for a function $\xi_0(x) \in \mathcal{D}(a,b)$and $\lambda_0 \in \mathbb{R}$, then the equation $(\check{f} - \lambda_0)\xi(x) = \xi_0(x)$ has a solution $\xi(x) \in \mathcal{D}(a,b)$.
3. The relation $\Phi_i(\check{f}\xi;z) = z\Phi_i(\xi;z)$ holds.

It follows from these properties that for any finite interval $\Delta \in \mathbb{R}$, there exists a set of functions $\{\xi_i(x) \in \mathcal{D}(a,b),\ i = 1,\dots,n\}$ such that

$$\det\left\|\Phi_i(\xi_j;\lambda)\right\| \neq 0,\ \ \forall\lambda \in \Delta. \tag{5.9}$$

In turn, this fact furnishes the following theorem.

Theorem 5.14. *Let $\hat{f}$ be an s.a. differential operator associated with an even s.a. differential operation $\check{f}$ of order n, and let $P(\lambda)$ be its IR. Let Δ be any finite interval of the real axis, and let a set of functions*

$$\{\xi_i(x) \in \mathcal{D}(a,b),\ i = 1,\dots,n\}$$

satisfy condition (5.9). Let functions $g_\Delta^{(i)}(x)$ be defined by

$$g_\Delta^{(i)}(x) = \int_\Delta \sum_{j=1}^{n} \Omega_{ij}(\lambda)\mathrm{d}P(\lambda)\xi_j(x),\ \ i = 1,\dots,n,$$

where the matrix $\Omega_{ij}(\lambda)$ is the inverse of the matrix $\Phi_i(\xi_j;\lambda)$ (it can be proved that the functions $g^{(i)}(x,\Delta)$ are actually independent of the choice of the functions ξ_j). Then for any function $\xi \in \mathcal{D}(a,b)$ and any interval $\Delta' \in \Delta$, the relation

$$\Pi(\Delta')\xi(x) = \int_{\Delta'} \sum_{i=1}^{n} \Phi_i(\xi;\lambda)\mathrm{d}P(\lambda)g_\Delta^{(i)}(x)$$

holds.

It follows from this theorem that $g_\Delta^{(i)}(x)$ as the functions of Δ form an improper generating basis of the operator $\hat{f}$, and therefore, the multiplicity of its spectrum does not exceed n.

5.3.2 Inversion Formulas, Green's Function, and Matrix Spectral Functions

A main consequence of Theorem 5.14 is the following theorem on inversion formulas.

Theorem 5.15. *Let $\sigma_{jk}(\lambda)$, $j,k = 1,\dots,n$, be a matrix spectral function given by (5.5) with the substitution $g_\Delta^{(j)}(x)$ for $\xi_{j,g}(\Delta)$. Then the formulas*

$$\eta(x) = \sum_{i,j=1}^{n} \int_{-\infty}^{\infty} \varphi_j(\lambda)u_k(x;\lambda)\mathrm{d}\sigma_{jk}(\lambda),\ \ \varphi_j(\lambda) = \int_a^b u_j(x;\lambda)\eta(x)\mathrm{d}x \quad (5.10)$$

establish an inverse isometric map $L^2(a,b) \Longleftrightarrow L^2_{n\sigma}$ with $\hat{f} \Longleftrightarrow \Lambda_\sigma$, so that the Parseval equality

$$\int_a^b |\eta(x)|^2\mathrm{d}x = \sum_{i,j=1}^{n} \int_{-\infty}^{\infty} \overline{\varphi_k(\lambda)}\varphi_j(\lambda)\mathrm{d}\sigma_{jk}(\lambda) \quad (5.11)$$

holds. The integrals in these formulas converge in the respective metrics of $L^2(a,b)$ and $L^2_{n\sigma}$.

The formulas (5.10) and (5.11) are called inversion formulas.

The theorem allows one to find spectral representations for integral kernels of the operators $\Pi(\Delta)$ and $\hat{\mathcal{R}}(z)$. One such representation is given and used below.

As is known, the resolvent $\hat{\mathcal{R}}(z)$ of any even s.a. differential operator $\hat{f}$ in $L^2(a,b)$ with $\operatorname{Im} z \neq 0$ is a bounded operator defined everywhere that allows the integral representation

$$\hat{\mathcal{R}}(z)\,\eta(x) = \int_a^b G(x,y;z)\eta(y)\mathrm{d}y,\ \forall\eta(x) \in L^2(a,b),$$

where the uniquely defined kernel $G(x,y;z)$ is called the *Green's function of an s.a. operator* $\hat{f}$; see [9, 116].

This means that there exists a one-to-one correspondence between the domain D_f of the operator $\hat{f}$ and the whole Hilbert space $L^2(a,b)$ given by

$$\left(\hat{f} - z\right)\xi(x) = \eta(x),\ \operatorname{Im} z \neq 0,\ \xi \in D_f,\ \eta \in L^2(a,b), \tag{5.12}$$

$$\xi(x) = \hat{\mathcal{R}}(z)\,\eta(x) = \int_a^b G(x,y;z)\eta(y)\mathrm{d}y. \tag{5.13}$$

It follows that a constructive way for evaluating the Green's function is to find a unique solution of (5.12) in integral form (5.13). Below, in Sect. 5.3.4, we discuss this possibility in detail.

It can be shown that if $\operatorname{Im} z \neq 0$, then one has the representation

$$\check{K}_x^{[k]}\check{K}_y^{[j]}\left[G(x,y;z) - G(x,y;\bar{z})\right] = (z-\bar{z})\sum_{l,m=1}^{n}\int_{-\infty}^{\infty}\frac{u_l^{[k]}(x;\lambda)u_m^{[j]}(y;\lambda)}{|z-\lambda|^2}\mathrm{d}\sigma_{ml}(\lambda), \tag{5.14}$$

where $\check{K}_x^{[k]}$ and $\check{K}_y^{[l]}$ are quasiderivatives of orders k and l in x and y respectively, and $k,l = 0,\dots,n-1$. The integrals in (5.14) are uniformly convergent with respect to both x and y in any square $\alpha \leq x, y \leq \beta$, $a < \alpha < \beta < b$. All the elements of the matrix function on the right-hand side of (5.14) are continuous in both x and y in any square $\alpha < x, y < \beta$.

We introduce the notation

$$M_{jk}(c;z) = \lim_{x\to c-0,\ y\to c+0}\check{K}_x^{[k-1]}\check{K}_y^{[j-1]}G(x,y;z),$$

$$\tilde{M}_{jk}(c;z) = \lim_{x\to c-0,\ y\to c+0}\check{K}_x^{[k-1]}\check{K}_y^{[j-1]}G(y,x;z),$$

$$\mu_{jk}(c;z) = \frac{1}{2i}\left[M_{jk}(c;z) - \overline{\tilde{M}_{jk}(c;z)}\right],\ j,k = 1,\dots,n. \tag{5.15}$$

Taking the limit $x \to c-0$ and $y \to c+0$ in representation (5.14) with due regard to the relation $G(x, y; \bar{z}) = \overline{G(y, x; z)}$ and normalization condition (5.8), we obtain the relation

$$\mu_{jk}(c; z) = \operatorname{Im} z \int_{-\infty}^{\infty} \frac{d\sigma_{jk}(\lambda)}{|z-\lambda|^2} . \tag{5.16}$$

Applying the Stieltjes inversion formula [9, 116] to (5.16), we obtain the following important representation for the matrix spectral function $\sigma_{jk}(\lambda)$:

$$\sigma_{jk}(\lambda) = \frac{1}{\pi} \lim_{\delta \to +0} \int_{\delta}^{\lambda+\delta} \mu_{jk}(c; \lambda' + i0) d\lambda', \tag{5.17}$$

where we take the normalization condition $\sigma_{jk}(0) = 0$ into account.

If an s.a. operator is real,[8] then its Green's function is symmetric, $G(x, y; z) = G(y, x; z)$ [9, 116]. In this case, we have $\tilde{M}_{jk}(c; z) = M_{jk}(c; z)$ and $\mu_{jk}(c; z) = \operatorname{Im} M_{jk}(c; z)$, and representation (5.17) becomes

$$\sigma_{jk}(\lambda) = \pi^{-1} \lim_{\delta \to +0} \int_{\delta}^{\lambda+\delta} \operatorname{Im} M_{jk}(c; \lambda' + i0) d\lambda'. \tag{5.18}$$

It follows from (5.18) that $\sigma_{jk}(\lambda)$ is real and is therefore symmetric, $\sigma_{jk}(\lambda) = \sigma_{kj}(\lambda)$. In all problems considered in this book, the Green's functions are really symmetric. In what follows, we therefore assume (5.18) for the spectral matrix function $\sigma_{jk}(\lambda)$.

In many cases, in particular, in all the specific cases considered in this book, the matrix spectral function is the sum of an a.c. matrix function with a positive semidefinite derivative on a certain interval $\Delta \in \mathbb{R}$ and a nondecreasing step function[9] with jumps at certain points λ_m, $m \in \mathcal{N} \subset \mathbb{Z}$.

In these cases, the derivative $\sigma'_{jk}(\lambda)$ treated in the sense of distributions is of the following structure:

$$\sigma'_{jk}(\lambda) = \pi^{-1} \operatorname{Im} M_{jk}(c; \lambda + i0) = \rho_{jk}(\lambda) + \sum_{m \in \mathcal{N}} \varkappa_{jk|m} \delta(\lambda - \lambda_m), \tag{5.19}$$

with a positive semidefinite matrix function $\rho_{jk}(\lambda)$ on an interval Δ and positive matrix coefficients $\varkappa_{jk|m} > 0$, so that spec $\hat{f} = \Delta \cup \{\lambda_m, \ m \in \mathcal{N}\}$. The points λ_m always can be numbered so that $\lambda_m \le \lambda_{m+1}$, $\forall m \in \mathcal{N}$.

---

[8] An operator $\hat{f}$ is called real if $\xi \in D_f$ implies that $\bar{\xi} \in D_f$ and $\hat{f}\xi = \eta$ implies that $\hat{f}\bar{\xi} = \bar{\eta}$.

[9] The spectral function generally can contain the so-called singular, or singular continuous, term; see [97]. Such terms are absent in all the cases encountered in this book.

If representation (5.19) holds, then the inversion formulas become

$$\eta(x)=\sum_{j,k=1}^{n}\int_{\Delta}\varphi_j(\lambda)\rho_{jk}(\lambda)u_k(x;\lambda)\mathrm{d}\lambda+\sum_{m\in\mathcal{N}}\sum_{j,k=1}^{n}\varphi_{j|m}\varkappa_{jk|m}u_k(x;\lambda_m),$$
$$\varphi_j(\lambda)=\int_a^b u_j(x;\lambda)\eta(x)\mathrm{d}x,\ \lambda\in\Delta,\ \varphi_{j|m}=\int_a^b u_j(x;\lambda_m)\eta(x)\mathrm{d}x,$$
$$\int_a^b|\eta(x)|^2\mathrm{d}x=\sum_{j,k=1}^{n}\int_{\Delta}\overline{\varphi_j(\lambda)}\rho_{jk}(\lambda)\varphi_k(\lambda)\mathrm{d}\lambda+\sum_{m\in\mathcal{N}}\sum_{j,k=1}^{n}\overline{\varphi_{j|m}}\varkappa_{jk|m}\varphi_{k|m}. \tag{5.20}$$

The integrals in (5.20) converge in the respective metrics of $L^2(a,b)$ and $L^2_{n\sigma}$.

5.3.3 Multiplicity of Spectrum; Simple Spectrum

Integrating in λ in (5.10) and (5.20) is in fact performed over the spectrum (over the set Gr_P of the matrix $\sigma(\lambda)$).

This means that the constancy points λ of the matrix $\sigma(\lambda)$ and the respective functions $u_i(x;\lambda)$ with such λ are not involved in the inversion formulas, so that the functions $u_i(x;\lambda)$ entering the integrands in the inversion formulas can be redefined by zero outside the spectrum points of the operator $\hat{f}$ (outside the growth points of the matrix $\sigma(\lambda)$). We note that in all known examples, the functions $u_i(x;\lambda)$ for λ that do not belong to the "mathematical" spectrum are eliminated by physical considerations, for example, because of their unrestricted growth at infinity for infinite intervals, while for finite intervals, they do not satisfy s.a. boundary conditions specifying the operator $\hat{f}$.

The inversion formulas represent a generalized Fourier expansion of any function belonging to the Hilbert space in terms of the functions $u_j(x;\lambda)$, $j=1,\dots,n$, which may not belong to the domain of the operator $\hat{f}$ or even to the Hilbert space.[10]

It is conventional to say that these functions form a complete system. But it may happen that for a given $\hat{f}$, there exists a complete system that contain a lesser number, say m, of functions, $m<n$.

It can be shown that for even s.a. differential operators considered in this book, the minimum m determines the multiplicity of the spectrum, so that the multiplicity of the spectrum does not exceed n. If $m=1$, the spectrum is simple; if $m>1$, the spectrum is m-fold.

[10]In such a situation, the functions $u_j(x;\lambda)$ are conventionally called the generalized eigenfunctions of the operator $\hat{f}$.

A qualitative explanation for the multiplicity of the spectrum to be less than n is as follows. Although all the functions $u_i(x;\lambda)$, $i = 1, \dots, n$, at a fixed λ formally are involved in inversion formulas (5.10) and (5.11), it may happen that in fact, they enter these formulas only via some linear combinations, and perhaps with zero coefficients. This is the case if the derivative of the matrix spectral function $\sigma'_{jk}(\lambda)$ is singular and its rank is equal to m for all λ belonging to the spectrum.[11]

For technical reasons, it is sometimes difficult to find the minimum complete system. In what follows, we formulate the conditions for the spectrum of $\hat{f}$ to be simple, i.e., conditions for a complete system to contain only one function $u(x;\lambda)$.

Definition 5.16. Let the following conditions hold: there exists a solution $u(x;z)$ of (5.7) that is real entire in z, and there exists a subspace $\mathbb{D}$ of functions $\xi(x) \in D_f$ that is dense in the Hilbert space, $\mathbb{D} \subset D_f$, $\overline{\mathbb{D}} = L^2(a,b)$, such that the guiding functional $\Phi(\xi;z)$ defined on $\mathbb{D}$ by (5.6) has the following properties:

(i) $\Phi(\xi;z)$ is entire in z for every $\xi(x) \in \mathbb{D}$.
(ii) If $\Phi(\xi_0;\lambda_0) = 0$ for a function $\xi_0(x) \in \mathbb{D}$ and $\lambda_0 \in \mathbb{R}$, then the equation $(\check{f} - \lambda_0)\psi(x) = \xi_0(x)$ has a solution $\psi(x) \in \mathbb{D}$.
(iii) For any $\xi(x) \in \mathbb{D}$, the relation $\Phi(\hat{f}\xi;z) = z\Phi(\xi;z)$ holds.

Then we call the functional $\Phi(\xi;z)$ a *simple guiding functional*.

We emphasize that a simple guiding functional for a given s.a. operator $\hat{f}$ exists iff an appropriate function u and subspace $\mathbb{D}$ exist.

One of the leading principles in constructing a simple guiding functional is to find a solution $u(x;z)$ with asymptotic behavior that coincides with the asymptotic behavior of functions belonging to D_f at one of the endpoints (a or b).

For the simple guiding functional $\Phi(\xi;z)$, analogues of Theorems 5.14 and 5.15 hold with the natural substitutions $i,j = 1$ and $g_\Delta(x)$, $\Phi(\xi;\lambda)$, $\Omega(\xi;\lambda)$, $\xi(x)$, $\varphi(\lambda)$, $u(x;\lambda)$, and $\sigma(\lambda)$ for the respective $g_\Delta^{(i)}(x)$, $\Phi_i(\xi;\lambda)$, $\Omega_{ij}(\xi;\lambda)$, $\xi_i(x)$, $\varphi_j(\lambda)$, $u_j(x;\lambda)$, and $\sigma_{jk}(\lambda)$, and $g_\Delta(x)$ as a function of Δ is an improper element of the operator $\hat{f}$. The existence of a simple guiding functional thus implies that the spectrum of the operator $\hat{f}$ is simple.

In the case of a simple spectrum, the matrix spectral function $\sigma_{jk}(\lambda)$ is reduced to a spectral function $\sigma(\lambda)$ that is given by (5.3) with the substitution $g_\Delta(x)$ for $\xi_g(\Delta)$ and can be evaluated in accordance with the following formulas:

$$\Sigma(c;\lambda) = \lim_{\delta\to+0} \pi^{-1} \int_\delta^{\lambda+\delta} \operatorname{Im} M(c;\lambda' + i0)\mathrm{d}\lambda',$$

$$\Sigma(c;\lambda) = \int_0^\lambda u^2(c;\lambda')\mathrm{d}\sigma(\lambda'),\ \ M(c;z) = G(c-0, c+0; z), \tag{5.21}$$

where c is a fixed inner point of the interval (a,b), $a < c < b$.

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[11] For some λ, it may be less than m.

The inversion formulas for an operator with simple spectrum are

$$\eta(x) = \int_{-\infty}^{\infty} \varphi(\lambda) u(x;\lambda) \mathrm{d}\sigma(\lambda)\,,\ \varphi(\lambda) = \int_a^b u(x;\lambda)\eta(x)\mathrm{d}x,$$
$$\int_a^b |\eta(x)|^2 \mathrm{d}x = \int_{-\infty}^{\infty} |\varphi(\lambda)|^2 \mathrm{d}\sigma(\lambda).$$

As was mentioned above, in all the problems considered in this book, the derivative of the matrix spectral function is of the form (5.19), which implies that in the case of a simple spectrum, the following general representation holds:

$$u^2(c;\lambda)\sigma'(\lambda) = \pi^{-1}\,\mathrm{Im}\, M(c;\lambda + i0)\,,$$
$$\sigma'(\lambda) = \rho^2(\lambda) + \sum_{m\in\mathcal{N}} \varkappa_m^2 \delta(\lambda - \lambda_m), \tag{5.22}$$

with a nonnegative function $\rho(\lambda)$ defined on an interval Δ, $\mathrm{supp}\,\rho = \Delta$, and some positive coefficients $\varkappa_m$, $\varkappa_m > 0$, so that $\mathrm{spec}\,\hat{f} = \Delta \cup \{\lambda_m,\ m \in \mathcal{N}\}$. The interval Δ determines the continuous part of the spectrum of $\hat{f}$, while the points λ_m determine its point spectrum.

If we introduce the normalized eigenfunctions $U_\lambda(x)$, $U_m(x)$ by

$$U_\lambda(x) = \rho(\lambda)u(x;\lambda),\ \lambda \in \Delta;$$
$$U_m(x) = \varkappa_m u(x;\lambda_m),\ m \in \mathcal{N},$$

the inversion formulas become

$$\eta(x) = \int_\Delta \phi(\lambda)U_\lambda(x)\mathrm{d}\lambda + \sum_{m\in\mathcal{N}} \phi_m U_m(x),$$
$$\phi(\lambda) = \int_a^b U_\lambda(x)\eta(x)\mathrm{d}x,\ \ \phi_m = \int_a^b U_m(x)\eta(x)\mathrm{d}x,$$
$$\int_a^b |\eta(x)|^2\mathrm{d}x = \int_\Delta |\phi(\lambda)|^2 \mathrm{d}\lambda + \sum_{m\in\mathcal{N}} |\phi_m|^2. \tag{5.23}$$

Using physics terminology and notation, we say that the system of eigenfunctions $\{U_\lambda(x),\ \ U_m(x)\}$ is complete in $L^2(a,b)$ and satisfies the orthogonality and completeness relations[12]

[12]For the continuous spectrum, these relations are symbolic in a sense.

$$\int_a^b U_\lambda(x)U_{\lambda'}(x)\mathrm{d}x = \delta(\lambda - \lambda'),\ \int_a^b U_\lambda(x)U_m(x)\mathrm{d}x = 0,$$
$$\int_a^b U_m(x)U_{m'}(x)\mathrm{d}x = \delta_{mm'},\ \lambda, \lambda' \in \Delta,\ m, m' \in \mathcal{N},$$
$$\int_\Delta U_\lambda(x)U_\lambda(y)\mathrm{d}\lambda + \sum_{m\in\mathcal{N}} U_m(x)U_m(y) = \delta(x - y). \tag{5.24}$$

In physics texts on QM, considerable effort is usually devoted to establishing just these relations.

5.3.4 Finding a Green's Function

Constructing integral representation (5.13) for a unique solution $\xi(x)$ of (5.12), and thereby finding the Green's function $G(x, y; z)$, proceeds in two steps.

The first step consists in finding the general solution of the inhomogeneous differential equation

$$\left(\check{f} - z\right)\xi(x) = \eta(x),\ \mathrm{Im}\, z \neq 0,\ \eta \in L^2(a, b) \tag{5.25}$$

using the method of variation of constants. According to this method, we seek a solution in the form

$$\xi(x) = \sum_{i=1}^{n} c_i(x)u_i(x; z), \tag{5.26}$$

where $u_i(x; z)$, $i = 1, \ldots, n$, is the fundamental system of solutions of the homogeneous equation

$$\left(\check{f} - z\right)u(x) = 0 \tag{5.27}$$

and $c_i(x)$, $i = 1, \ldots, n$, are some unknown functions subject to the conditions

$$\sum_{i=1}^{n} u_i^{[k-1]}(x; z)c_i'(x) = 0,\ k = 1, \ldots, n-1,\ c_i'(x) = d_x c_i(x)\,. \tag{5.28}$$

Substituting representation (5.26) into (5.25) and taking conditions (5.28) into account, we obtain the equation

$$\sum_{i=1}^{n} u_i^{[n-1]}(x; z)c_i'(x) = -\eta(x)\,. \tag{5.29}$$

Equations (5.28) and (5.29) together form the system of linear algebraic equations

$$\sum_{i=1}^{n} \mathbb{W}_{ki}(x;z)c_i'(x) = -\eta_k(x)\,,\ k = 1,\ldots,n,$$
$$\eta_k(x) = \delta_{kn}\eta(x),\ \mathbb{W}_{ki}(x;z) = u_i^{[k-1]}(x;z) \tag{5.30}$$

for the derivatives $c_i'(x)$ of the desired coefficient functions. The determinant of the matrix $\mathbb{W}_{ki}(x;z)$ in (5.30) is the quasi-Wronskian $\mathbb{W}\mathrm{r}\,(u_1,\ldots,u_n)$ of the fundamental system of solutions of homogeneous equation (5.27). The quasi-Wronskian is independent of x and is different from zero, and therefore, system (5.30) has a unique solution:

$$c_i'(x) = \sum_{k=1}^{n}\left[\mathbb{W}^{-1}(x;z)\right]_{ik}\eta_k(x) = -v_i(x;z)\eta(x),$$
$$v_i(x;z) = \left[\mathbb{W}^{-1}(x;z)\right]_{in}.$$

The functions $v_i(x;z)$ can be shown to satisfy the homogeneous equation (5.27) and therefore can be represented as linear combinations of the solutions $u_i(x;z)$, $i = 1,\ldots,n$, of the fundamental system. The general solution of (5.25) finally is given by

$$\xi(x) = \sum_{i=1}^{n}\left[c_i u_i(x;z) - u_i(x;z)\int_{x_0}^{x} v_i(y;z)\eta(y)\mathrm{d}y\right], \tag{5.31}$$

where c_i are arbitrary constants, and x_0 is a fixed inner point of the interval (a,b).

As an illustration, we consider the case of an s.a. differential operation of second order ($n = 2$)

$$\check{f} = -d_x\left[p_0(x)d_x\right] + p_1(x),$$

which is important from the standpoint of further applications.

In this case, we have

$$\check{K}_x^{[0]} = 1,\ \check{K}_x^{[1]} = p_0(x)d_x,\ \check{K}_x^{[2]} = p_1(x) - d_x\check{K}_x^{[1]} = \check{f},$$

and the fundamental system of solutions of the homogeneous equation (5.27) consists of two functions $u_i(x;z)$, $i = 1,2$. The matrices $\mathbb{W}$ and $\mathbb{W}^{-1}$ are given by

$$\mathbb{W} = \begin{pmatrix} u_1 & u_2 \\ u_1^{[1]} & u_2^{[1]} \end{pmatrix},\ \mathbb{W}^{-1} = \omega^{-1}\begin{pmatrix} u_2^{[1]} & -u_2 \\ -u_1^{[1]} & u_1 \end{pmatrix},$$

where

$$\omega = \mathbb{W}\mathrm{r}(u_1,u_2) = u_1u_2^{[1]} - u_1^{[1]}u_2 = \mathrm{const}.$$

The functions v_i, $i = 1, 2$, are $v_1 = -u_2/\omega$ and $v_2 = u_1/\omega$, so that the general solution of the inhomogeneous equation (5.25) reads

$$\xi(x) = \sum_{i=1}^{2} c_i u_i(x; z) + \omega^{-1} \int_{x_0}^{x} [u_1(x; z)u_2(y; z) - u_2(x; z)u_1(y; z)]\, \eta(y)\mathrm{d}y, \tag{5.32}$$

where c_1, c_2 are some constants.

The second step in finding the Green's function consists in taking the condition $\xi \in D_f$ on the solution of (5.12) into account, which leads to determining the constants c_i, $i = 1, \dots, n$, in (5.31) as linear functionals in η; the condition $\xi \in D_f$ means that $\xi(x)$ belongs to $L^2(a, b)$ and satisfies the s.a. boundary conditions specifying the s.a. operator $\hat{f}$. This results in integral representation (5.13) for the resolvent and thereby in the Green's function.

5.3.5 Matrix Operators

We here present a spectral analysis scheme for s.a. 2×2 matrix operators in the Hilbert space $\mathbb{L}^2(\mathbb{R}_+) = L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$. Such operators emerge as certain radial Hamiltonians in Chaps. 8 and 9. A specific feature of these radial Hamiltonians is that their spectra are simple, so that it suffices to consider only one simple guiding functional.

A guiding functional $\Phi(F; z)$ for an s.a. 2×2 matrix operator $\hat{h}_\mathfrak{e}$ associated with an s.a. 2×2 matrix differential operation $\check{h}$ and acting in the space of doublets $F(r) = (f \diagup g) \in \mathbb{L}^2(\mathbb{R}_+)$ is given by

$$\Phi(F; z) = \int_{\mathbb{R}_+} U(r; z)F(r)\mathrm{d}r, \quad F \in \mathbb{D} = D_r(\mathbb{R}_+) \cap D_{h_\mathfrak{e}},$$
$$U(r) = (u \diagup v), \; U(r; z)F(r) = uf + vg, \tag{5.33}$$

where the doublet U is a solution of the homogeneous equation $(\check{h} - z)U(r; z) = 0$ that is real entire in z and satisfies s.a. boundary conditions at the left end (the origin) specifying the s.a. operator $\hat{h}_\mathfrak{e}$. By definition, the functional (5.33) is simple if it has the following properties:

1. $\Phi(F; z)$ is entire in z for every $F(r)$.
2. If $\Phi(F_0; \lambda_0) = 0$ for a doublet $F_0(r) \in \mathbb{D}$ and $\lambda_0 \in \mathbb{R}$, then the equation $\left(\check{h} - \lambda_0\right) \Psi(r) = F_0(r)$ has a solution $\Psi \in \mathbb{D}$.
3. For any $F(r) \in \mathbb{D}$, the relation $\Phi(\hat{h}_\mathfrak{e} F; z) = z\Phi(F; z)$ holds.

In all the problems considered in Chaps. 8 and 9, the doublet U satisfies required s.a. boundary conditions, and the corresponding guiding functional (5.33) is simple.

It follows that the spectrum of the Hamiltonian $\hat{h}_{\mathfrak{e}}$ is simple and there exists a spectral function $\sigma(\lambda)$, $\lambda \in \mathbb{R}$, that determines the inversion formulas for this operator (see below). The derivative[13] $\sigma'(\lambda)$ of the spectral function, $\sigma'(\lambda) \geq 0$, is related to the Green's function of the operator $\hat{h}_{\mathfrak{e}}$ by

$$U(c;\lambda) \otimes U(c;\lambda)\sigma'(\lambda) = \pi^{-1} \operatorname{Im} G(c-0, c+0; \lambda + i0),$$

where c is an arbitrary internal point of the interval $\mathbb{R}_+$, and $\sigma'(\lambda)$ is independent of c.

In addition, $\sigma'(\lambda)$ is of the structure

$$\sigma'(\lambda) = \rho^2(\lambda) + \sum_{n \in \mathcal{N}} Q_n^2 \delta(\lambda - \lambda_n)$$

with a nonnegative function $\rho(\lambda)$, $\rho(\lambda) \geq 0$, and some positive coefficients Q_n, $Q_n > 0$; the support Δ of the function $\rho(\lambda)$, $\Delta = \operatorname{supp} \rho$, is the continuous part of the spectrum of the operator $\hat{h}_{\mathfrak{e}}$, while the points λ_n determine its point spectrum, so that spec $\hat{h}_{\mathfrak{e}} = \Delta \cup \{\lambda_n,\ n \in \mathcal{N}\}$.

The matrix Green's function $G(r, r'; z)$ is the integral kernel of the resolvent of the s.a. matrix operator $\hat{h}_{\mathfrak{e}}$. To find the Green's function with $\operatorname{Im} z > 0$, we have to represent a unique solution $F(r) \in D_{h_{\mathfrak{e}}}$ of the differential equation

$$(\check{h} - z)F(r) = \Psi(r),\ \forall \Psi \in \mathbb{L}^2(\mathbb{R}_+), \tag{5.34}$$

in the integral form

$$F(r) = \int_{\mathbb{R}_+} G(r, r'; z)\Psi(r')\mathrm{d}r'. \tag{5.35}$$

The normalized (generalized) eigendoublets $U_\lambda(r) = \rho(\lambda)U(r;\lambda)$, $\lambda \in \Delta$, of $\hat{h}_{\mathfrak{e}}$ corresponding to the continuous spectrum, and normalized eigendoublets $U_n(x) = Q_n U(r;\lambda_n)$, $n \in \mathcal{N}$, corresponding to the discrete spectrum form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$. This means that the following inversion formulas hold:

$$F(r) = \int_\Delta \varphi(\lambda)U_\lambda(r)\mathrm{d}\lambda + \sum_{n \in \mathcal{N}} \varphi_n U_n(r),$$

$$\varphi(\lambda) = \int_{\mathbb{R}_+} U_\lambda(r)F(r)\mathrm{d}r\,,\quad \varphi_n = \int_{\mathbb{R}_+} U_n(r)F(r)\mathrm{d}r\,,$$

$$\int_{\mathbb{R}_+} |F(r)|^2\mathrm{d}r = \int_\Delta |\phi(\lambda)|^2\mathrm{d}\lambda + \sum_{n \in \mathcal{N}} |\phi_n|^2. \tag{5.36}$$

[13]Treated in the sense of distributions.

5.4 Appendix

5.4.1 Some Simple Guiding Functionals

In most problems considered in the subsequent chapters, spectra of s.a. operators are simple. Moreover, a choice of guiding functionals and a proof of their simplicity are quite similar and can be reduced to five typical cases, which we consider in detail in this section. All the cases have common features described just below and differ only in s.a. boundary conditions listed in items A, B, C, D, E in Sect. 5.4.1.2. In what follows, when solving spectral problems where simple guiding functionals fall into one of these cases, we refer to this subsection and to the corresponding item. We first describe common features inherent in each of the cases. We consider s.a. differential operators $\hat{f}_{\mathfrak{e}}$ in $L^2(a,b)$, where (a,b) are various intervals with a finite left endpoint, $|a| < \infty$. Each operator $\hat{f}_{\mathfrak{e}}$ is associated with an s.a. Schrödinger differential operation $\check{f} = -d_x^2 + V(x)$ on the interval (a,b), where the potential $V(x)$ is a smooth function in the interval,[14] and its domain $D_{f_{\mathfrak{e}}}$ is specified by split s.a. boundary conditions.[15] According to Theorem 4.24, the latter means that the asymptotic behavior of functions $\psi \in D_{f_{\mathfrak{e}}} \subseteq D^*_{\check{f}}(a,b)$ at the endpoints of the interval is given by (4.120) and the diagonal a.b. coefficients $\{c_{\pm,k}\}_1^m$ are related by (4.124), or (4.125), where the matrix U is of the form (4.126). For our purposes, it is convenient to change $U(a)$ to $U^+(a)$ and to take the matrix U in the form

$$U = \operatorname{diag}(U(b), U^+(a)),\ U(b) = U_{lk}(b),\ l,k = 1,\dots,\ p_+(b) = p_-(b),$$
$$U(a) = U_{lk}(a),\ l,k = p_+(b)+1,\dots,p_+(b)+p_-(a),\ p_+(a) = p_-(a),$$

where $U(b)$ is a unitary $p_+(b)\times p_+(b)$ matrix and $U(a)$ is a unitary $p_+(a)\times p_+(a)$ matrix, so that the split s.a. boundary conditions become

$$c_{-,l}(b) = \sum_{l=1}^{p_+(b))} U_{lk}(b)c_{+,k}(b),\ l = 1,\dots,p_+(b), \tag{5.37}$$

$$c_{-,l}(a) = \sum_{l=1}^{p_+(a).} U_{lk}(a)c_{+,k}(a),\ l = 1,\dots,p_+(a). \tag{5.38}$$

It may be that $p_+(b) = 0$, which is equivalent to vanishing of the right boundary form, $[\psi_*, \psi_*](b) \equiv 0$; in such a case, s.a. boundary conditions are reduced to (5.38). A similar remark also refers to the endpoint a.

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[14] That is, the potential can be singular only at the endpoints of the interval.

[15] We note that possible mixed s.a. boundary conditions, like periodic ones, are beyond the scope of our consideration in this section, although such boundary conditions can yield a simple spectrum.

For guiding functionals in all the cases, we take the functionals $\Phi(\xi; z)$ defined on the domains $\mathbb{D} = D_r(a,b) \cap D_{f_\mathfrak{e}}$ dense in $L^2(a,b)$ and given by

$$\Phi(\xi; z) = \int_a^b U(x; z)\xi(x)\mathrm{d}x, \ \xi \in \mathbb{D} \tag{5.39}$$

(a unique functional in each case),[16] where $U(x; z)$ is a solution of the homogeneous equation

$$(\check{f} - z)U(x; z) = 0, \tag{5.40}$$

which is smooth in (a,b) as a function of x at any fixed z, real entire in z at any fixed inner point x of (a,b), and satisfies the following properties:

(a) $U(x; z)$ is continuous as a function of two variables in any open restricted region $O \subset (a,b) \otimes \mathbb{C}$; it is also evident that the function $U_\eta(x; z) = \eta(x)U(x; z)$, where $\eta(x)$ is a smooth function given by

$$\eta(x) = 1, \ x \in [a, a_0]; \ \eta(x) = 0, \ x \in [b_0, b]; \ a < a_0 < b_0 < b,$$

belongs to $D_{f_\mathfrak{e}}$.

(b) $U(x; z)$ has an asymptotic behavior at the left endpoint a given by (4.120) and satisfies boundary conditions (5.38).

In what follows, we examine whether the above-introduced functionals have the properties (i), (ii), and (iii) defining a simple guiding functional in Sect. 5.3.3 and show that under some special additional conditions relevant to the properties (i) and (ii), they have, and therefore, the spectra of the operators $\hat{f}_\mathfrak{e}$ prove to be simple, which allows us to establish the inversion formulas for $\hat{f}_\mathfrak{e}$. An interesting remark is in order. It is remarkable that boundary conditions at the right endpoint b are not involved even if they are nontrivial. They enter the final result for the (generalized) eigenfunctions via the Green's functions, which take these conditions into account, and the respective spectral functions.

We begin with property (iii), whose proof is simplest.

5.4.1.1 Property (iii)

By definition (5.39), we have

$$\Phi(\hat{f}_\mathfrak{e}\xi; z) = \int_a^b U(x; z)\check{f}\xi(x)\mathrm{d}x.$$

Using the integral Lagrange identity (4.16) and (5.40) for $U(x; z)$, we obtain

$$\Phi(\hat{f}_\mathfrak{e}\xi; z) = z\Phi(\xi; z) + [U, \xi]_a^b .$$

[16] Which is sufficient if the functional proves to be simple.

But the right boundary form $[U, \xi](b)$ vanishes because every $\xi \in \mathbb{D}$ is equal to zero in a neighborhood of the right endpoint b, while the left boundary form $[U, \xi](a)$ vanishes because both $U(x; z)$ and $\xi(x)$ have a similar asymptotic behavior at the left endpoint a given by (4.120) and satisfy boundary conditions (5.38) with the same matrix $U(a)$, which yields $\Phi(\hat{f}_{\mathfrak{e}}\xi; z) = z\Phi(\xi; z)$, the required property (iii).

As for properties (i) and (ii), we can prove them under certain additional specific conditions on the asymptotic behavior of the functions $\psi \in D_{f_{\mathfrak{e}}}$ and the respective functions $U(x, z)$ at the left endpoint a. We distinguish five different cases of the asymptotic behavior (see the items A, B, C, D, E below).

We continue with the property (ii).

5.4.1.2 Property (ii)

Let

$$\Phi(\xi_0; \lambda_0) = \int_a^b U(x; \lambda_0)\xi_0(x)\mathrm{d}x = \int_a^\beta U(x; \lambda_0)\xi_0(x)\mathrm{d}x = 0$$

for some $\lambda_0 \in \mathbb{R}$ and some $\xi_0 \in \mathbb{D}$, $\mathrm{supp}\xi_0 \in [a, \beta]$, $\beta < b$, and let $\tilde{U}(x)$ be a solution of (5.40) with $z = \lambda_0$ that is linearly independent of $U(x; \lambda_0)$, so that $\omega = -\mathrm{Wr}(U, \tilde{U}) \neq 0$. We consider a particular solution $\psi(x)$ of the equation $(\check{f} - \lambda_0)\psi(x) = \xi_0(x)$ that is given by[17]

$$\begin{aligned}
\psi(x) &= \frac{1}{\omega}\left[U(x; \lambda_0)\int_x^\beta \tilde{U}(x)\xi_0(x)\mathrm{d}x + \tilde{U}(x)\int_a^x U(x; \lambda_0)\xi_0(x)\mathrm{d}x\right], \\
\psi'(x) &= \frac{1}{\omega}\left[U'(x; \lambda_0)\int_x^\beta \tilde{U}(x)\xi_0(x)\mathrm{d}x + \tilde{U}'(x)\int_a^x U(x; \lambda_0)\xi_0(x)\mathrm{d}x\right].
\end{aligned} \tag{5.41}$$

The function (5.41) has the following evident properties: ψ is correctly defined on (a, b), and ψ and ψ' are a.c. in (a, b); $\mathrm{supp}\psi \in [a, \beta]$, and therefore, ψ is square-integrable on any interval (c, b), $c > a$, and trivially satisfies boundary conditions (5.37) at the right endpoint b (the respective a.b. coefficients $c_{\pm,k} = 0$). If we can prove that ψ is square-integrable at the left endpoint a, i.e., is square-integrable on an interval $[a, c]$, $a < c < b$, we will prove that $\psi \in L^2(a, b)$ and $\check{f}\psi = \lambda_0\psi + \xi_0 \in L^2(a, b)$. If in addition we prove that ψ satisfies boundary conditions (5.38) at the left endpoint,[18] we will prove that $\psi \in D_{f_{\mathfrak{e}}}$ and therefore (because

[17]See the representation (5.32) for the general solution of such an equation in the end of Sect. 5.3.3 with the substitutions $\xi \to \psi$, $u_1 \to U$, and $u_2 \to \tilde{U}$.

[18]We note that a preliminary estimate of the asymptotic behavior of the function ψ (5.41) at the left endpoint a may be sufficient to assert that $\psi \in L^2(a, b)$.

$\operatorname{supp}\psi \in [a,\beta]$, $\beta < b$) $\psi \in \mathbb{D}$, which means that the guiding functional $\Phi(\xi; z)$ (5.39) has the property (ii).

We don't know a general method for evaluating the asymptotic behavior of the function $\psi(x)$ (5.41) at the left endpoint a for arbitrary $\check{f}$, i.e., for arbitrary potentials $V(x)$. But for our further purposes, it is sufficient to consider five special cases labeled A, B, C, D, and E, which we examine separately below.

We introduce the notation $\delta = x - a$ and represent the asymptotic behavior of the relevant functions at the left endpoint a, as $\delta \to 0$, in terms of δ.

A. Let $\mu \geq 1$, and let the asymptotics of the relevant functions as $\delta \to 0$ be given by[19]

$$\begin{gathered}
U(x;z) = \delta^{1/2+\mu} + O(\delta^{3/2+\mu}),\ U'(x;z) = (1/2+\mu)\delta^{-1/2+\mu} + O(\delta^{1/2+\mu}),\\
\tilde{U}(x) = \delta^{1/2-\mu} + O(\delta^{3/2-\mu}),\ \tilde{U}'(x) = (1/2-\mu)\delta^{-1/2-\mu} + O(\delta^{1/2-\mu}),\\
\xi(x) = \begin{cases} O(\delta^{3/2}),\ \mu > 1,\\ O(\delta^{3/2}\sqrt{\ln\delta}),\ \mu = 1, \end{cases} \qquad \xi'(x) = \begin{cases} O(\delta^{1/2}),\ \mu > 1,\\ O(\delta^{1/2}\sqrt{\ln\delta}),\ \mu = 1. \end{cases}
\end{gathered} \tag{5.42}$$

We represent the function $\psi(x)$ (5.41) as

$$\begin{aligned}
\psi(x) = cU(x;\lambda_0) + \omega^{-1}\Bigg[U(x;\lambda_0)\int_x^{x_0}\tilde{U}(x)\xi_0(x)\mathrm{d}x\\
+\tilde{U}(x;\lambda_0)\int_a^x U(x)\xi_0(x)\mathrm{d}x\Bigg],\quad c = \omega^{-1}\int_{x_0}^{\beta}\tilde{U}(x)\xi_0(x)\mathrm{d}x,
\end{aligned} \tag{5.43}$$

where $x_0 > a$ is a fixed point such that $\delta_0 = x_0 - a$ is small enough to use asymptotics (5.42) for estimating the integral terms on the right-hand side of (5.43) by means of the Cauchy–Schwarz inequality. Performing the estimates, we obtain

$$\psi(x) = \begin{cases} O(\delta^{1/2+\mu}),\ 1 \leq \mu < 3,\\ O(\delta^{7/2}\ln\delta),\ \mu = 3,\\ O(\delta^{7/2}),\ \mu > 3, \end{cases} \qquad \delta \to 0,$$

which in particular means that ψ is square-integrable at the endpoint a. In a similar way, we obtain

$$\psi'(x) = \begin{cases} O(\delta^{-1/2+\mu}),\ 1 \leq \mu < 3,\\ O(\delta^{5/2}\ln\delta),\ \mu = 3,\\ O(\delta^{5/2}),\ \mu > 3, \end{cases} \qquad \delta \to 0.$$

[19]This is the case in which $p_+(a) = p_-(a) = 0$, i.e., the left a.b. coefficients are equal to zero.

These estimates show that the asymptotic behavior of the function $\psi(x)$ (5.41) is within the limits (5.42) for the asymptotic behavior of the functions $\xi(x)$, whence it follows that $\psi \in \mathbb{D}$, which proves property (ii) in case A.

B. Let $0 < \mu < 1$, let $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, and let the asymptotics of the relevant functions as $\delta \to 0$ be given by[20]

$$
\begin{aligned}
U(x;z) &= u_{B\mathrm{as}}(x) + O(\delta^{2-|1/2-\mu|}),\\
U'(x;z) &= u'_{B\mathrm{as}}(x) + O(\delta^{1-|1/2-\mu|}),\\
u_{B\mathrm{as}}(x) &= (\kappa_0\delta)^{1/2+\mu}\cos\nu + u_{2B\mathrm{as}}(x)\sin\nu,\\
\tilde{U}(x) &= (\kappa_0\delta)^{1/2+\mu}\sin\nu - u_{2B\mathrm{as}}(x)\cos\nu + O(\delta^{5/2-\mu}),\\
\tilde{U}'(x) &= (1/2+\mu)(\kappa_0\delta)^{-1/2+\mu}\sin\nu - u'_{2B\mathrm{as}}(x)\cos\nu + O(\delta^{3/2-\mu}),\\
\xi(x) &= c_\xi u_{B\mathrm{as}}(x) + O(\delta^{3/2}),\ \xi'(x) = c_\xi u'_{B\mathrm{as}}(x) + O(\delta^{1/2}),\\
u_{2B\mathrm{as}}(x) &= (\kappa_0\delta)^{1/2-\mu} + c_1(\kappa_0\delta)^{3/2-\mu},
\end{aligned}
\tag{5.44}
$$

where κ_0 and c_1 are some constants and c_ξ is an arbitrary constant.[21] We represent the function $\psi(x)$ (5.41) as

$$
\begin{aligned}
\psi(x) = cU(x;\lambda_0) + \omega^{-1}\Big[\tilde{U}(x)\int_a^x U(x;\lambda_0)\xi_0(x)\mathrm{d}x \\
-U(x;\lambda_0)\int_a^x \tilde{U}(x)\xi_0(x)\mathrm{d}x\Big],\ \ c = \omega^{-1}\int_a^\beta \tilde{U}(x)\xi_0(x)\mathrm{d}x.
\end{aligned}
\tag{5.45}
$$

A similar representation holds for $\psi'(x)$. These representations allow us to establish the asymptotics of $\psi(x)$ and $\psi'(x)$ as $\delta \to 0$ to yield

$$
\begin{aligned}
\psi(x) &= cu_{B\mathrm{as}}(x) + O(\delta^{5/2-\mu}),\\
\psi'(x) &= cu'_{B\mathrm{as}}(x) + O(\delta^{3/2-\mu}),
\end{aligned}
$$

which implies that $\psi(x)$ is square-integrable at the left endpoint a and satisfies s.a. boundary condition (5.44) at this endpoint. It follows that $\psi \in \mathbb{D}$, which proves property (ii) in case B.

C. Let the asymptotics of the relevant functions as $\delta \to 0$ be given by

$$
\begin{aligned}
U(x;z) &= u_{C\mathrm{as}}(x) + O(\delta^{3/2}\ln\delta),\\
\tilde{U}(x) &= (\kappa_0\delta)^{1/2}\sin\nu - u_{2C\mathrm{as}}(x)\cos\nu + O(\delta^{3/2}\ln\delta),
\end{aligned}
$$

[20] This is the case in which $p_+(a) = p_-(a) = 1$.

[21] The constant κ_0 is of dimension of inverse length, so that $\kappa_0\delta$ is dimensionless.

$$\xi(x) = c_\xi u_{C\,\mathrm{as}}(x) + O(\delta^{3/2}\ln\delta),$$
$$u_{C\,\mathrm{as}}(x) = (\kappa_0\delta)^{1/2}\cos\nu + u_{2C\,\mathrm{as}}(x)\sin\nu,$$
$$u_{2C\,\mathrm{as}}(x) = (\kappa_0\delta)^{1/2}\ln(\kappa_0\delta) + c_2(\kappa_0\delta)^{1/2}, \tag{5.46}$$

where κ_0 and c_2 are some constants and c_ξ is an arbitrary constant, and let the asymptotics of the functions U', $\tilde{U}'$, and ξ as $\delta \to 0$ be given by the derivatives of respective asymptotics (5.46). Using representation (5.45) for the function $\psi(x)$ (5.41) and a similar representation for $\psi'(x)$ and estimating the integral terms in these representations by means of the Cauchy–Schwarz inequality, we obtain

$$\psi(x) = cu_{C\,\mathrm{as}}(x) + O(\delta^{5/2}\ln^2\delta),$$
$$\psi'(x) = cu'_{C\,\mathrm{as}}(x) + O(\delta^{3/2}\ln^2\delta),\ \delta \to 0,$$

which implies that $\psi(x)$ is square-integrable at the left endpoint a and satisfies s.a. boundary condition (5.46) at this endpoint. It follows that $\psi \in \mathbb{D}$, which proves property (ii) in case C.

D. Let $\mu = i\varkappa,\ \varkappa > 0$, and let the asymptotics of the relevant functions as $\delta \to 0$ be given by[22]

$$U(x;z) = u_{D\,\mathrm{as}}(x) + O(\delta^{3/2}),$$
$$\tilde{U}(x) = \mathrm{e}^{\mathrm{i}\theta}(\kappa_0\delta)^{1/2+i\varkappa} - \mathrm{e}^{-\mathrm{i}\theta}(\kappa_0\delta)^{1/2-i\varkappa} + O(\delta^{3/2}),$$
$$\xi(x) = c_\xi u_{D\,\mathrm{as}}(x) + O(\delta^{3/2}),$$
$$u_{D\,\mathrm{as}}(x) = \mathrm{e}^{\mathrm{i}\theta}(\kappa_0\delta)^{1/2+i\varkappa} + \mathrm{e}^{-\mathrm{i}\theta}(\kappa_0\delta)^{1/2-i\varkappa}, \tag{5.47}$$

where κ_0 is some constant and c_ξ is an arbitrary constant, and let the asymptotics of the functions U', $\tilde{U}'$, and ξ as $\delta \to 0$ be given by the derivatives of respective asymptotics (5.47). Using representation (5.45) for the function $\psi(x)$ (5.41) and a similar representation for $\psi'(x)$ and estimating the corresponding integral terms by means of the Cauchy–Schwarz inequality, we obtain

$$\psi(x) = cu_{D\,\mathrm{as}}(x) + O(\delta^{5/2}),$$
$$\psi'(x) = cu'_{D\,\mathrm{as}}(x) + O(\delta^{3/2}),\ \delta \to 0,$$

which implies that $\psi(x)$ is square-integrable at the left endpoint a and satisfies s.a. boundary condition (5.47) at this endpoint. It follows that $\psi \in \mathbb{D}$, which proves property (ii) in case D.

E. Let the left endpoint a be regular, and let the asymptotic behavior of the relevant functions as $\delta \to 0$ be given by

[22]This is the case in which $p_+(a) = p_-(a) = 1$.

$$U(x;z) = u_{E\mathrm{as}}(x) + O(\delta^2),\ u_{E\mathrm{as}}(x) = \cos\nu + \kappa_0\delta\sin\nu,$$
$$\tilde{U}(x) = \sin\nu - \kappa_0\delta\cos\nu + O(\delta^2),\ \xi(x) = c_\xi u_{B\mathrm{as}}(x) + O(\delta^{3/2}),$$

where $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, κ_0 is some constant, and c_ξ is an arbitrary constant.

A proof of property (ii) in this case is completely similar to that in the case B with $\mu = 1/2$.

It remains to prove property (i) for the guiding functional $\Phi(\xi; z)$ (5.39) in the above cases A, B, C, D, and E.

5.4.1.3 Property (i)

We recall that the function $U(x;z)$ has the following properties[23]: as a function of x, it is smooth in (a, b) for any $z \in \mathbb{C}$, but can be singular at the endpoints of the interval, and as a function of z, it is (real) entire for any inner point $x \in (a, b)$.

In the cases A, C, D, and E, the function $U(x;z)$ has a finite limit at the left endpoint a, which implies that it is entire in z for any $x \in [a, \beta]$, $\forall\beta < b$, and is bounded as a function of two variables in $[a, \beta] \times O$, where O is any bounded region in $\mathbb{C}$. Let D be any circle in $\mathbb{C}$ of finite radius, and let Γ be its boundary. As an entire function in z, the function $U(x;z)$ allows the contour integral representation

$$U(x;z) = \frac{1}{2\pi i}\oint_\Gamma \frac{U(x;\zeta)}{\zeta - z} d\zeta,\ z \in D \setminus \Gamma.$$

Then for any $\xi \in \mathbb{D}$ with $\mathrm{supp}\xi \subseteq [a, \beta]$, the guiding functional $\Phi(\xi; z)$ (5.39) allows the representation

$$\Phi(\xi; z) = \frac{1}{2\pi i}\int_a^\beta \mathrm{d}x \left[\oint_\Gamma \mathrm{d}\zeta \frac{U(x;\zeta)\xi(x)}{\zeta - z}\right],\ z \in D \setminus \Gamma, \tag{5.48}$$

where the integral is an iterated one. But in the cases A, C, D, and E, the function $(\zeta - z)^{-1}U(x;\zeta)\xi(x)$ is bounded and is therefore integrable on $[a, \beta] \times \lneqq$. It then follows from Fubini's theorem [97] that the order of integration on the right-hand side of (5.48) can be interchanged, and the representation becomes

$$\Phi(\xi; z) = \frac{1}{2\pi i}\oint_\Gamma \mathrm{d}\zeta \frac{1}{\zeta - z}\left[\int_a^\beta \mathrm{d}x U(x;\zeta)\xi(x)\right],\ z \in D \setminus \Gamma. \tag{5.49}$$

The representation (5.49) demonstrates that $\Phi(\xi; z)$ is an analytic function in z in the circle D and is therefore entire in z because D is arbitrary.

---

[23] By the function $U(x;z)$, we here mean the specific function U for each operator $\hat{f}_{\mathfrak{e}}$.

In case B, the function $U(x;z)$ is generally singular[24] at the left endpoint a, but allows the representation

$$U(x;z) = u_{B\mathrm{as}}(x) + U_{(1)}(x;z),$$

where $u_{B\mathrm{as}}(x)$ is generally singular at a, but is independent of z, while $U_{(1)}(x;z) = O(\delta^{2-|1/2-\mu|})$ as $\delta = x-a \to 0$. Accordingly, the guiding functional $\Phi(\xi;z)$ (5.39) is represented as a sum of two functionals

$$\Phi(\xi;z) = \Phi_{\mathrm{as}}(\xi) + \Phi_{(1)}(\xi;z) = \int_a^b \mathrm{d}x u_{B\mathrm{as}}(x)\xi(x) + \int_a^b \mathrm{d}x U_{(1)}(x;z)\xi(x),$$

where the first functional $\Phi_{\mathrm{as}}(\xi)$ is trivially entire in z, while for the second functional $\Phi_{(1)}(\xi;z)$, we can repeat all the previous arguments proving that $\Phi_{(1)}(\xi;z)$ is entire in z because the function $U_{(1)}(x;z)$ repeats all the required properties of the previous function $U(x;z)$. Therefore, property (i) also holds in case B.

A summary of this subsection is that in the above cases A, B, C, D, and E, the functional $\Phi(\xi;z)$ (5.39) is a simple guiding functional.

5.4.2 A Useful Lemma

When solving spectral problems, we often encounter expressions of the form $\operatorname{Im}\omega^{-1}(E+i0)$, $E \in \mathbb{R}$.

For a certain class of functions $\omega(W)$ of a complex variable W, such limits allow a convenient representation in terms of distributions based on the Sokhotsky formula

$$\operatorname{Im}(x+i0)^{-1} = -\pi\delta(x). \tag{5.50}$$

Lemma 5.17. *Let $\omega(W)$ be an analytic function of W in a region U such that $U \cap \mathbb{R} = U_0 \neq \varnothing$, and let $\omega(W)$ have only one simple root $E_0 \in U_0$, so that $\omega(E_0) = 0$, $\omega'(E_0) \neq 0$, and $\operatorname{Im}\omega'(E_0) = 0$. Then*

$$\operatorname{Im}\omega^{-1}(E+i0) = Q\delta(E-E_0) + \rho(E),\ Q = -\pi\left[\omega'(E_0)\right]^{-1},$$

$$\rho(E) = \begin{cases} \operatorname{Im}\omega^{-1}(E),\ E \neq E_0, \\ \operatorname{Im}\omega^{-1}(E_0 \pm 0),\ E = E_0, \end{cases} \qquad E \in U_0\,.$$

[24]Namely, for $\mu > 1/2$ and $\nu \neq \pm\pi/2$.

In particular, if $\operatorname{Im}\omega(E) = 0$, $\forall E \in U_0$, *then*

$$\operatorname{Im}\omega^{-1}(E + i0) = Q\delta(E - E_0),\ Q = -\pi\left[\omega'(E_0)\right]^{-1},\ E \in U_0.$$

Proof. Introducing the notation $\Delta = W - E_0$ and $a = \omega'(E_0)$, we represent the function $\omega(W)$ as $\omega(W) = a\Delta + b(W)\Delta^2$ and the function $\omega^{-1}(W)$ respectively as

$$\omega^{-1}(W) = a^{-1}\Delta^{-1} + c(W),\ c(W) = -\frac{b(W)}{a[a + b(W)\Delta]},$$

where $c(W)$ is continuous in U. With due regard to the Sokhotsky formula, it immediately follows from this representation that

$$\operatorname{Im}\omega^{-1}(E + i0) = -\pi a^{-1}\delta(E - E_0) + \operatorname{Im}c(E),\ E \in U_0,$$

where

$$\operatorname{Im}c(E) = \operatorname{Im}\omega^{-1}(E),\ E \neq E_0,$$
$$\operatorname{Im}c(E_0) = -a^{-2}\operatorname{Im}b(E_0) = \operatorname{Im}\omega^{-1}(E_0 \pm 0).$$

□

As an illustration, we evaluate two limits, $\operatorname{Im}\Gamma(X(E + i0))$ and $\operatorname{Im}\psi(X(E + i0))$, where ψ is the logarithmic derivative of the Γ function, and

$$X(E + i\varepsilon) = -n + c(\Delta + i\varepsilon),\ n \in \mathbb{Z}_+,\ c = \overline{c},\ \Delta = E - E_0,\ E_0 \in \mathbb{R},\ |c\Delta| < 1.$$

In the case of the first limit, we have $\omega(W) = \Gamma^{-1}(X(W))$. It is well known that $\Gamma^{-1}(X)$ is real entire in X, whence $\omega(W)$ is real entire in W and evidently satisfies the conditions of the lemma including the additional condition $\operatorname{Im}\omega(E) = 0$. Therefore, to find the first limit, we have only to evaluate $\omega'(E_0)$, for which it is sufficient to estimate the behavior of $\omega(E)$ near the root point up to Δ^2. Using the representation

$$\Gamma^{-1}(X) = \pi^{-1}\Gamma(1 - X)\sin(\pi X),$$

we obtain that $\omega(E) = (-1)^n cn!\Delta + O(\Delta^2)$ and find that

$$\operatorname{Im}\Gamma(X(E + i0)) = (-1)^{n+1}\frac{\pi}{cn!}\delta(E - E_0).$$

Similar arguments with a certain modification are applicable to the case of the second limit, where we have $\omega(W) = \Gamma(X(W))[\Gamma'(X(W))]^{-1}$. The difference with the previous case is that the function $\omega(W)$ is real meromorphic with poles at certain real points where $\Gamma'(X)$ vanishes. But we note that in the regions under consideration, $\operatorname{Im}\psi(X) = 0$ for $\Delta \neq 0$, and therefore, it is sufficient to consider only a neighborhood of the root point E_0 where the lemma is applicable. By virtue of the same representation for $\Gamma(X)$, the behavior of $\omega(E)$ near the root point is given by $\omega(E) = -c\Delta + O(\Delta^2)$, which yields

$$\operatorname{Im}\psi(X(E + i0)) = \pi c^{-1}\delta(E - E_0).$$

Chapter 6
Free One-Dimensional Particle on an Interval

Based on the general considerations in Chaps. 3, 4, and 5, we here consider s.a. extensions and spectral problems for the momentum and Hamiltonian for a free one-dimensional nonrelativistic particle moving on an interval (a, b). It turns out that the solution of these problems crucially depends on the type of the interval: whether it is the whole real axis, $(a, b) = \mathbb{R}$, or a semiaxis, $(a, b) = \mathbb{R}_+$ (a is taken to be zero for convenience; it can be any finite number), or $(a, b) = \mathbb{R}_-$, or a finite interval, $-\infty < a < b < \infty$; without loss of generality, we always consider a finite interval $[0, l]$, $l < \infty$.

For the space of states of the system, we conventionally take the Hilbert space $L^2(a, b)$, whose vectors are wave functions $\psi(x)$, $x \in (a, b)$ (we use the x-representation). In Sect. 6.1, we discuss the momentum operator on different intervals. The Hamilton operator is discussed in Sect. 6.2. In Sect. 6.3, we discuss in detail how the correct treatment removes all the paradoxes presented in Sect. 1.3. In the present chapter, with the exception of Sect. 6.3, we set $\hbar = 1$.

6.1 Self-adjoint Extensions and Spectral Problem for the Momentum Operator

To construct an s.a. momentum operator, we start with the corresponding differential operation $\check{p} = -i d_x$ (4.6), which follows from the formal canonical quantization in the coordinate representation; see Chap. 1. We next construct the initial symmetric operator $\hat{p}$, its adjoint $\hat{p}^+$, and possible s.a. extensions of $\hat{p}$. All these operators differ by their domains, whereas each of them acts on the corresponding domain by the same differential operation $\check{p}$. That is why we only indicate the domains of these operators in what follows.

The domain of the initial symmetric operator $\hat{p}$ is the space $\mathcal{D}(a, b)$ of smooth functions with compact support, $D_p = \mathcal{D}(a, b)$. The operator $\hat{p}$ is evidently symmetric: the boundary forms $[\chi, \psi](a/b)$ are trivial because all the functions belonging to $\mathcal{D}(a, b)$ vanish in a neighborhood of the boundaries.

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It is instructive to directly evaluate the adjoint $\hat{p}^{+}$, although such a problem was solved for the initial symmetric operator associated with the general s.a. differential operation in Sect. 4.4.

We have to solve the defining equation

$$(\chi, \varphi) - (\psi_*, \hat{p}\varphi) = \int_a^b \mathrm{d}x \left(\overline{\chi}\varphi + i\overline{\psi_*}\varphi'\right) = 0,\ \forall\varphi \in \mathcal{D}(a,b), \tag{6.1}$$

for pairs $\psi_* \in D_{p^+}$ and $\chi = \hat{p}^{+}\psi_*$. Let a pair ψ_* and χ be a solution of defining equation (6.1). We represent the function $\chi(x)$ as

$$\chi(x) = -i\tilde{\psi}'(x),\ \tilde{\psi}(x) = i\int_c^x \mathrm{d}y\chi(y), \tag{6.2}$$

where the point c is an interior point or a finite (regular) endpoint of the interval (a,b). By definition, the function $\tilde{\psi}(x)$ is a.c. Substituting representation (6.2) for χ into (6.1) and integrating by parts, we reduce (6.1) to the equation

$$\int_a^b \mathrm{d}x\overline{\left(\psi_* - \tilde{\psi}\right)}\varphi' = 0,\ \forall\varphi \in \mathcal{D}(a,b)$$

(the boundary terms vanish because of vanishing φ near the boundaries). Applying Lemma 2.12, we conclude that $\psi_* - \tilde{\psi} = C = \text{const}$, or

$$\psi_*(x) = i\int_c^x \mathrm{d}y\chi(y) + C, \tag{6.3}$$

whence it follows that ψ_* is a.c. in (a,b) and $\chi = \check{p}\psi_* = -i\psi_*'$. Conversely, any pair ψ_* and χ of functions belonging to $L^2(a,b)$ and satisfying relation (6.3) evidently satisfies defining equation (6.1). Therefore, $D_{p^+} = D^*_{\check{p}}(a,b)$.

To check the symmetricity of $\hat{p}^{+}$, we consider the quadratic asymmetry form $\Delta_{p^+}(\psi_*)$ (3.10) of this operator. According to (4.36), (4.37), it is represented in terms of the quadratic boundary forms $[\psi_*, \psi_*](a/b)$ as

$$\Delta_{p^+}(\psi_*) = [\psi_*, \psi_*](x)|_a^b,\ \ [\psi_*, \psi_*](x) = -i\overline{\psi_*(x)}\psi_*(x). \tag{6.4}$$

In the case of $(a,b) = \mathbb{R}$, the boundary forms $[\psi_*, \psi_*](\pm\infty)$ are trivial, see below, and therefore, the operator $\hat{p}^{+}$ is symmetric.

In the case that one or both endpoints of an interval (a,b) are finite, for example, $|a| < \infty$ and/or $|b| < \infty$, we generally have $[\psi_*, \psi_*](a) \neq 0$ and/or $[\psi_*, \psi_*](b) \neq 0$, which implies that the operator $\hat{p}^{+}$ is not symmetric.

The deficient subspaces and deficiency indices of the operator $\hat{p}$ are determined by solutions of the differential equations

$$\check{p}\psi_{\pm}(x) = -i\psi_{\pm}'(x) = \pm i\kappa\psi_{\pm}(x), \tag{6.5}$$

where κ is an arbitrary, but fixed, parameter of dimension of inverse length. The respective general solutions of these equations are

$$\psi_{\pm}(x) = c_{\pm}\mathrm{e}^{\mp\kappa x}, \tag{6.6}$$

where $c_{\pm}$ are some constants.

From this point on, our consideration depends on the type of interval. We first consider the whole real axis.

6.1.1 Whole Real Axis

The Hilbert space of states for a particle on the whole real axis is $\mathfrak{H} = L^2(\mathbb{R})$. The domain of the initial symmetric operator $\hat{p}$ is $D_p = \mathcal{D}(\mathbb{R})$, while the domain of its adjoint $\hat{p}^+$ is $D_{p^+} = D^*_{\check{p}}(\mathbb{R})$. The functions ψ_* belonging to $D^*_{\check{p}}(\mathbb{R})$ satisfy the conditions $\psi_*, \psi'_* \in L^2(\mathbb{R})$ and therefore vanish at infinity, see Lemma 2.13, which implies that the quadratic boundary forms are trivial, $[\psi_*, \psi_*](\pm\infty) = 0$. It follows that quadratic asymmetry form (6.4) is zero and the operator $\hat{p}^+$ is therefore symmetric. This means that the operator $\hat{p}$ is essentially s.a., and its unique s.a. extension, we let $\hat{p}_{\mathfrak{e}}$ denote it, is its closure coinciding with its adjoint, $\hat{p}_{\mathfrak{e}} = \overline{\hat{p}} = \hat{p}^+$.

An alternative argument for the validity of this assertion is the general standard one. The solutions (6.6) of (6.5) are both non-square-integrable on the whole axis, ψ_+ is non-square-integrable at $-\infty$, while ψ_- is at ∞. This means that the deficiency indices of the operator $\hat{p}$ are zero, and therefore this operator is essentially s.a.

Thus there exists only one s.a. momentum operator $\hat{p}_{\mathfrak{e}}$ on the whole axis.

As we know from Chaps. 2 and 5, the spectrum of any s.a. operator is on the real axis. We now prove that the spectrum of the s.a. momentum operator $\hat{p}_{\mathfrak{e}}$ is the whole axis, $\operatorname{spec}\hat{p}_{\mathfrak{e}} = \mathbb{R}$.

Assume the contrary. Suppose a point $\lambda_0 \in \mathbb{R}$ does not belong to $\operatorname{spec}\hat{p}_{\mathfrak{e}}$, i.e., the point λ_0 is a regular point of the operator $\hat{p}_{\mathfrak{e}}$. This means that the operator $(\hat{p}_{\mathfrak{e}} - \lambda_0)^{-1}$ is defined on the whole of $L^2(\mathbb{R})$ (see the definition of a regular point in Sect. 5.1), or the equation

$$(\check{p} - \lambda_0)\xi = \eta \tag{6.7}$$

with any $\eta \in L^2(\mathbb{R})$ has a (unique) solution $\xi \in D^*_{\check{p}}(\mathbb{R})$. Let $\operatorname{supp}\eta \in (\alpha, \beta)$, $-\infty < \alpha < \beta < \infty$. The general solution of differential equation (6.7) is

$$\xi(x) = \mathrm{e}^{i\lambda_0 x}\left[i\int_{\alpha}^{x} \mathrm{d}y\mathrm{e}^{-i\lambda_0 y}\eta(y) + C\right],$$

where C is an arbitrary constant. For $x < \alpha$, we have $\xi(x) = C\mathrm{e}^{i\lambda_0 x}$, and the condition $\xi \in L^2(\mathbb{R})$ requires that $C = 0$. For $x > \beta$, we then have

$$\xi(x) = C_1(\eta)\mathrm{e}^{i\lambda_0 x},\;\; C_1(\eta) = i\int_{\alpha}^{\beta} \mathrm{d}y\mathrm{e}^{-i\lambda_0 y}\eta(y),$$

and the condition $\xi \in L^2(\mathbb{R})$ requires that $C_1(\eta) = 0$. But it is easy to present functions $\eta \in L^2(\mathbb{R})$ for which $C_1(\eta) \neq 0$, for example, $\eta(x) = \mathrm{e}^{i\lambda_0 x}\varphi(x)$, $\varphi(x) > 0$, which implies that for such functions, (6.7) has no square-integrable solutions. This contradiction proves that spec $\hat{p}_{\mathfrak{e}} = \mathbb{R}$.

The operator $\hat{p}_{\mathfrak{e}}$ has no eigenvectors. Again, assume the contrary. Let a function $U_\lambda(x)$ be an eigenfunction of the operator $\hat{p}_{\mathfrak{e}}$ corresponding to an eigenvalue $\lambda \in \mathbb{R}$. By definition, this function is a square-integrable solution of the equation $U'_\lambda(x) = i\lambda U_\lambda(x)$. But the general solution of this equation is

$$U_\lambda(x) = C \exp(i\lambda x)\,,\ C \in \mathbb{C}, \tag{6.8}$$

which is not square-integrable for any $\lambda \in \mathbb{R}$ and $C \neq 0$. This contradiction proves that $\hat{p}_{\mathfrak{e}}$ has no point spectrum, and its spectrum is pure continuous; see Chap. 5.

However, it is well known that functions (6.8) form a complete orthonormalized system in $L^2(\mathbb{R})$; they are therefore called the generalized eigenfunctions. Namely, inversion formulas (5.23) with $U_\lambda(x) = (2\pi)^{-1/2}\exp(i\lambda x)$ and $U_n = 0$, which are well known as Fourier transformations, hold,

$$\eta(x) = \int_{\mathbb{R}} \phi(\lambda)U_\lambda(x)\mathrm{d}\lambda,\ \phi(\lambda) = \int_{\mathbb{R}} U_\lambda(x)\eta(x)\mathrm{d}x,\ \forall\eta \in L^2(\mathbb{R}). \tag{6.9}$$

As was mentioned in Chap. 5, the integrals in the inversion formulas converge in the sense of the metrics of the respective Hilbert spaces. We illustrate this point with the above transformations.

As an example, we consider the first integral in (6.9). This integral has to be understood as follows. We introduce the functions $\eta_N(x)$ defined by

$$\eta_N(x) = \begin{cases} \eta(x),\ -N \le x \le N, \\ 0,\ |x| > N. \end{cases}$$

Their Fourier transforms are

$$\phi_N(\lambda) = (2\pi)^{-1/2}\int_{-\infty}^{\infty} \mathrm{d}x\mathrm{e}^{i\lambda x}\eta_N(x),\ \phi_N(\lambda) \in L^2_\lambda(\mathbb{R})\,.$$

It is evident that $\{\eta_N(x)\}$ is a Cauchy sequence and that it converges to the vector $\eta(x)$ as $N \to \infty$. Due to the equality

$$\|\phi_{N_2} - \phi_{N_1}\|^2 = \|\eta_{N_2} - \eta_{N_1}\|^2,$$

$\{\phi_N(\lambda)\}$ is also a Cauchy sequence. Because the space $L^2_\lambda(\mathbb{R})$ of functions of the variable λ is complete, the sequence $\{\phi_N(\lambda)\}$ converges to a vector $\phi(\lambda)$ as $N \to \infty$.

6.1.2 A Semiaxis

The Hilbert space of states is the space $L^2(\mathbb{R}_+)$. The domains of the initial symmetric operator $\hat{p}$ and its adjoint $\hat{p}^+$ are respectively $D_p = \mathcal{D}(\mathbb{R}_+)$ and $D_{p^+} = D^*_{\check{p}}(\mathbb{R}_+)$.

It is useful to evaluate the closure $\overline{\hat{p}}$ of the operator $\hat{p}$ using the relation $\overline{\hat{p}} = \left(\hat{p}^+\right)^+$; see Chap. 3. In that chapter, it was demonstrated that the domain $D_{\overline{p}}$ of the operator $\overline{\hat{p}}$ consists of functions $\underline{\psi} \in D^*_{\check{p}}(\mathbb{R}_+)$ that satisfy the additional condition $\omega_{p^+}(\psi_*, \underline{\psi}) = 0$, $\forall \psi_* \in D^*_{\check{p}}(\mathbb{R}_+)$; see (3.12). In the case under consideration, $\psi_* \overset{x\to\infty}{\longrightarrow} 0$, so that the latter condition becomes

$$\overline{\psi_*(0)}\underline{\psi}(0) = 0, \ \forall \psi_* \in D^*_{\check{p}}(\mathbb{R}_+) \Longrightarrow \underline{\psi}(0) = 0,$$

and we obtain

$$D_{\overline{p}} = \{\underline{\psi} : \underline{\psi} \in D^*_{\check{p}}(\mathbb{R}_+), \ \ \underline{\psi}(0) = 0\}. \tag{6.10}$$

We now turn to the deficient subspaces of the operator $\hat{p}$. They are determined by the same solutions (6.6) of the differential equations (6.5) reduced to the semiaxis $\mathbb{R}_+$. The function ψ_+ is square-integrable on $\mathbb{R}_+$, whereas ψ_- is not. This means that the deficient subspaces of the initial symmetric operator $\hat{p}$ on the semiaxis are $D_+ = \{ce_+\}$, $e_+ = \mathrm{e}^{-\kappa x}$, $c \in \mathbb{C}$, and $D_- = \{0\}$ and its deficiency indices are $(1, 0)$.

We come to the same conclusion considering the quadratic form $\Delta_{p^+}(\psi_*)$, $\psi_* \in D^*_{\check{p}}(\mathbb{R}_+)$.

Indeed, the right boundary form is trivial, $[\psi_*, \psi_*](\infty) = 0$. The left endpoint of the semiaxis is regular, and the left boundary form is nontrivial, $[\psi_*, \psi_*](0) = -i\,|\psi_*(0)|^2 \neq 0$, because in general, $\psi_*(0) \neq 0$.

The boundary value $\psi_*(0)$ plays the role of a unique asymptotic boundary coefficient.

The Hermitian form $(1/i)\,\Delta_{p^+}(\psi_*) = |\psi_*(0)|^2$ is a positive semidefinite form in this boundary value, its inertia indices, and therefore the deficiency indices of the initial symmetric operator $\hat{p}$, are evidently equal to $(1, 0)$. We note that we obtain this result without finding the deficient subspaces.

The unequal deficiency indices imply that there are no s.a. extensions of the initial symmetric operator $\hat{p}$ associated with the differential operation $\check{p}$ on the semiaxis $\mathbb{R}_+$. In the language of physics, this means that for a particle moving on the semiaxis, the notion of momentum as a QM observable is lacking. In particular, there is no notion of radial momentum.

Although the operator $\hat{p}$ has no s.a. extensions, we can find some closed extensions of $\hat{p}$ such that their adjoints are also the extensions of $\hat{p}$: if we let $\hat{g}$ denote such an extension, then $\hat{p} \subseteq \hat{g} = \overline{\hat{g}}$ and $\hat{p} \subseteq \hat{g}^+$. We show that there are only two such extensions, $\hat{g}_1 = \overline{\hat{p}}$ and $\hat{g}_2 = \hat{p}^+$. Indeed, because $\overline{\hat{p}}$ is the minimum closed extension of $\hat{p}$, we have $\overline{\hat{p}} \subseteq \hat{g} = \overline{\hat{g}}$ and $\overline{\hat{p}} \subseteq \hat{g}^+$. Taking the adjoints of these two inclusions and using the relation $(\hat{g}^+)^+ = g$, we obtain that $\overline{\hat{p}} \subseteq \hat{g} \subseteq \hat{p}^+$and $\overline{\hat{p}} \subseteq \hat{g}^+ \subseteq \hat{p}^+$. In the case under consideration, the first von Neumann formula (4.44) becomes

$$D_{p^+} = D^*_{\check{p}}(\mathbb{R}_+) = D_{\overline{p}} + D_+ = D_{\overline{p}} + \{ce_+\},$$

and therefore, the domain D_g of $\hat{g}$ coincides either with $D_{\overline{p}}$ or with D_{p^+}.

6.1.3 A Finite Interval

6.1.3.1 Self-adjoint Momentum Operator

The Hilbert space of states is $L^2(0,l)$. The domains of the initial symmetric operator $\hat{p}$ and its adjoint $\hat{p}^+$ are respectively $D_p = \mathcal{D}(0,l)$ and $D_{p^+} = D^*_{\check{p}}(0,l)$.

The functions $\psi_\pm$ in (6.6) are square-integrable on a finite interval, which implies that the deficient subspaces of the operator $\hat{p}$ are one-dimensional subspaces $D_\pm = \{c_\pm e_\pm, c_\pm \in \mathbb{C}\}$, where $e_+ = \mathrm{e}^{-\kappa x}$ and $e_- = \mathrm{e}^{-\kappa(l-x)}$ are the respective basis vectors of the same norm, so that the initial symmetric operator $\hat{p}$ on a finite interval has the equal deficiency indices $m_\pm = 1$. By the main theorem, Theorem 3.4, there exists a one-parameter family $\{\hat{p}_U,\ U \in U(1)\}$ of s.a. extensions of $\hat{p}$ (the group $U(1)$ is a circle $\left\{\mathrm{e}^{i\theta},\ \theta \in \mathbb{S}(0,2\pi)\right\}$). We consider both ways of specification of s.a. extensions given by the main theorem and a third, alternative, way of directly finding s.a. boundary conditions, which is given by Theorem 4.24.

The first way requires evaluating the closure $\overline{\hat{p}}$, which reduces to finding its domain $D_{\overline{p}}$. The equivalent defining equations for $\underline{\psi} \in D_{\overline{p}}$ are given in (3.13) and in (3.16) or (3.17). We use the defining equation in (3.13), which in our case is $\omega_{p^+}(\psi_*, \underline{\psi}) = 0,\ \forall \psi_* \in D^*_{\check{p}}(0,l)$. This equation reduces to the equation

$$\overline{\psi_*(l)}\underline{\psi}(l) - \overline{\psi_*(0)}\underline{\psi}(0) = 0\,,\ \forall \psi_* \in D^*_{\check{p}}(0,l)\,,$$

for the boundary values of functions $\underline{\psi}$ belonging to $D_{\overline{p}}$. Because $\psi_*(0)$ and $\psi_*(l)$ can take arbitrary values independently, which in particular follows from representation (6.3), we obtain that $\underline{\psi}(0) = \underline{\psi}(l) = 0$. We arrive at the same result considering defining equation (3.17) for $D_{\overline{p}}$ because the determinant of the boundary values of the basis vectors $e_\pm$ is nonzero,

$$\det\begin{pmatrix} e_+(l) & e_+(0) \\ e_-(l) & e_-(0) \end{pmatrix} = \mathrm{e}^{-2\kappa l} - 1 \neq 0.$$

Therefore, the functions $\underline{\psi} \in D_{\overline{p}}$ are specified as the functions belonging to $D^*_{\check{p}}(0,l)$ and satisfying the additional zero boundary conditions

$$D_{\overline{p}} = \left\{\underline{\psi} : \underline{\psi} \in D^*_{\check{p}}(0,l)\,;\ \underline{\psi}(0) = \underline{\psi}(l) = 0\right\}.$$

Isometries $\hat{U} : D_{+} \longmapsto D_{-}$ are determined by complex numbers of unit modulus, $\hat{U}(\theta)\, e_{+} = \mathrm{e}^{i\theta} e_{-}$, and are labeled by an angle $\theta \in \mathbb{S}(0, 2\pi)$. Respectively, the one-parameter $U(1)$ family $\{\hat{p}_{\theta}\}$ of s.a. extensions of $\hat{p}$ is given by the domains

$$D_{p_\theta} = \left\{\psi_\theta : \psi_\theta = \underline{\psi} + c\left(\mathrm{e}^{-\kappa x} + \mathrm{e}^{i\theta - \kappa(l-x)}\right),\ \underline{\psi} \in D_{\overline{p}}\right\}, \tag{6.11}$$

where c is an arbitrary constant.

The second way of specifying s.a. extensions of $\hat{p}$ requires solving the defining equation $\omega_{p^+}\left(e_{+} + \mathrm{e}^{i\theta} e_{-}, \psi_\theta\right) = 0$ for functions ψ_θ belonging to D_{p_θ}; see (3.33) or (3.35). In our case, this equation reduces to

$$\left[e_{+} + \mathrm{e}^{i\theta} e_{-}, \psi_\theta\right]\Big|_0^l = -i\left(\mathrm{e}^{-\kappa l} + \mathrm{e}^{-i\theta}\right)\psi_\theta(l) + i\left(1 + \mathrm{e}^{-i\theta - \kappa l}\right)\psi_\theta(0) = 0.$$

Its solution is the relation

$$\psi_\theta(l) = \mathrm{e}^{i\vartheta}\psi_\theta(0)\,,\quad \vartheta = \theta - 2\arctan\left(\frac{\sin\theta}{\mathrm{e}^{\kappa l} + \cos\theta}\right), \tag{6.12}$$

between the boundary values of the functions belonging to D_{p_θ}. The angle ϑ ranges from 0 to 2π as θ ranges from 0 to 2π, $\vartheta \in \mathbb{S}(0, 2\pi)$, and is in one-to-one correspondence with the angle θ (it is sufficient to show that $\vartheta(\theta)$ is a monotonic function, $\mathrm{d}\vartheta/\mathrm{d}\theta > 0$); therefore, the angle ϑ equivalently labels the $U(1)$ family of s.a. extensions, which we write as $\hat{p}_\vartheta = \hat{p}_\theta$.

The domain $D_{p_\vartheta} = D_{p_\theta}$ of the momentum operator $\hat{p}_\vartheta = \hat{p}_\theta$ consists of functions $\psi_\vartheta = \psi_\theta$ that belong to $D^*_{\check{p}}(0, l)$ and satisfy the additional boundary condition (6.12). This boundary condition is an s.a. boundary condition specifying the s.a. extensions of the initial symmetric operator $\check{p}$:

$$D_{p_\vartheta} = \left\{\psi_\vartheta : \psi_\vartheta \in D^*_{\check{p}}(0, l)\,;\ \ \psi_\vartheta(l) = \mathrm{e}^{i\vartheta}\psi_\vartheta(0)\right\}. \tag{6.13}$$

It is easy to verify that representation (6.12) is equivalent to representation (6.11).

The second way of specifying s.a. extensions appears to be more direct and explicit than the first one[1] because it specifies s.a. extensions in the customary form of s.a. boundary conditions, which is more suitable for spectral analysis.

And finally, we can use the third way, the asymmetry form method given by Theorem 4.24. Namely, we impose the condition $\Delta_{p^+}(\psi_*) = -i\,\overline{\psi_*}(x)\,\psi_*(x)\big|_0^l = 0$ to reduce the domain $D^*_{\check{p}}(0, l)$ of the adjoint operator $\hat{p}^+$ to the domain of an s.a. momentum operator, which directly yields the s.a. boundary conditions

$$\psi_\vartheta(l) = \mathrm{e}^{i\vartheta}\psi_\vartheta(0)\,,\ \vartheta \in \mathbb{S}(0, 2\pi)\,, \tag{6.14}$$

and reproduces the result (6.13) without evaluating the deficient subspaces.

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[1] Although in the general formulation of Theorem 3.4, the situation seems to be the opposite.

A conclusion of the above consideration is that for a particle moving on a finite interval, the momentum operator is defined nonuniquely. There exists a one-parameter $U(1)$ family $\{\hat{p}_\vartheta\}$ of s.a. operators associated with the differential operation $\check{p}$, labeled by an angle ϑ, and specified by s.a. boundary conditions (6.14). Each $\hat{p}_\vartheta$ can be considered the momentum operator for a particle moving on a finite interval.

As in the previous case of a semiaxis, we find all closed extensions $\hat{g}$ of $\hat{p}$, $\hat{g} = \overline{\hat{g}}$, such that their adjoints $\hat{g}^+$ are also the extensions of $\hat{p}$. In perfect analogy with the previous case, these requirements imply that the following inclusions hold: $\overline{\hat{p}} \subseteq \hat{g} \subseteq \hat{p}^+$ and $\overline{\hat{p}} \subseteq \hat{g}^+ \subseteq \hat{p}^+$, which is equivalent to that both $\hat{g}$ and $\hat{g}^+$ are associated with the differential operation $\check{p}$ and their domains are restricted by

$$D_{\overline{p}} \subseteq D_g \subseteq D^*_{\check{p}}(0,l)\,, \quad D_{\overline{p}} \subseteq D_{g^+} \subseteq D^*_{\check{p}}(0,l)\,.$$

By the first von Neumann formula (4.44) as applied to our case, we have

$$D^*_{\check{p}}(0,l) = D_{\overline{p}} + D_+ + D_- = D_{\overline{p}} + \{c_+e_+\} + \{c_-e_-\}.$$

It follows from this representation and the above inclusions that for any extension $\hat{g}$, its domain D_g allows the representation $D_g = D_{\overline{p}} + \Delta D_g$, where ΔD_g is a subspace of the direct sum of the deficient subspaces, $\Delta D_g \subseteq D_+ + D_-$; the same holds for the adjoint $\hat{g}^+$: $D_{g^+} = D_{\overline{p}} + \Delta D_{g^+}$, $\Delta D_{g^+} \subseteq D_+ + D_-$. Because $D_+ + D_-$ is two-dimensional, there are three possibilities for ΔD_g:

(1) The minimum ΔD_g is the zero subspace of $D_+ + D_-$, $\Delta D_g = \{0\}$, in which case $\hat{g} = \hat{g}_1 = \overline{\hat{p}}$ and $\hat{g}^+ = \hat{p}^+$.
(2) The maximum ΔD_g is two dimensional and coincides with the whole of $D_+ + D_-$, $\Delta D_g = D_+ + D_-$, in which case $\hat{g} = \hat{g}_2 = \hat{p}^+$ and $\hat{g}^+ = \overline{\hat{p}}$.
(3) An intermediate ΔD_g is a one-dimensional subspace of the two-dimensional sum $D_+ + D_-$. There is the two-parameter family $\{\Delta D_{(\nu)} = \Delta D_{(\alpha,\theta)}\}$ of such one-dimensional subspaces determined by basis vectors

$$\nu = \nu(\alpha,\vartheta) = e_+ \sin\alpha + \mathrm{e}^{i\vartheta} e_- \cos\alpha\,,\; 0 \le \alpha \le \pi/2,\; 0 \le \vartheta \le 2\pi,$$

so that $\Delta D_{(\nu)} = \{c\nu\}$, $c \in \mathbb{C}$, which generates the two-parameter family $\{\hat{g}_{(\nu)} = \hat{g}_{(\alpha,\theta)}\}$ of the required closed extensions of $\hat{p}$ such that

$$D_{g_{(\nu)}} = D_{g_{(\alpha,\theta)}} = D_{\overline{p}} + \Delta D_{(\nu)} = D_{\overline{p}} + c(e_+ \sin\alpha + \mathrm{e}^{i\theta} e_- \cos\alpha\,).$$

The adjoint $\hat{g}^+_{(\nu)}$, i.e., its domain $D_{g^+_{(\nu)}}$, can be evaluated using defining equation (2.24), which is reduced to the equation $(\chi, \hat{g}_{(\nu)}\psi) = (\hat{g}^+_{(\nu)}\chi, \psi)$, $\forall\psi \in D_{g_{(\nu)}}$, for $\chi \in D_{g^+_{(\nu)}}$. It is evident from the equality $(\hat{g}^+)^+ = \hat{g}$ and the previous two items that $D_{g^+_{(\nu)}} = D_{\overline{p}} + \Delta D_{g^+_{(\nu)}}$, where the subspace $\Delta D_{g^+_{(\nu)}} \subseteq D_+ + D_-$ is also one-dimensional, $\Delta D_{g^+_{(\nu)}} = \Delta D_{(\tilde{\nu})} = \Delta D_{(\beta,\theta)} = c(e_+ \sin\beta + \mathrm{e}^{i\theta} e_- \cos\beta)$. Because both $\hat{g}_{(\nu)}$ and $\hat{g}^+_{(\nu)}$ are restrictions of $\hat{p}^+$, the defining equation is equivalent to the equation $\omega_{p^+}(\chi,\psi) = 0, \forall\psi \in D_{g_{(\nu)}}$. In view of the von Neumann formula (4.45) and the equality $\|e_+\| = \|e_-\|$, this equation reduces to $\sin\beta \sin\alpha - \mathrm{e}^{-i(\vartheta-\theta)} \cos\beta \cos\alpha = 0$ (of course, the same result follows from the representation of $\omega_{p^+}(\chi,\psi)$ in terms of boundary forms). The solution of the latter equation is $\vartheta = \theta$ and $\beta = \pi/2 - \alpha$, so that

$$D_{g^+_{(\nu)}} = D_{g^+_{(\alpha,\theta)}} = D_{\overline{p}} + c(e_+ \cos\alpha + \mathrm{e}^{i\theta} e_- \sin\alpha).$$

We note that all the s.a. operators $\hat{p}_\theta$ (6.11) represent a part of the above family, $\hat{p}_\theta = \hat{g}_{\pi/4,\theta}$. In addition, the property $\hat{g}_{\alpha,\theta} = \hat{g}^+_{\pi/2-\alpha}$ holds, and the operators $\hat{g}_{0,\theta}$, $\hat{g}^+_{0,\theta}$, $\hat{g}_{\pi/2,\theta}$, and $\hat{g}^+_{\pi/2,\theta}$ do not depend on θ.

6.1.3.2 Spectrum and Inversion Formulas

We begin with the spectra of the s.a. operators $\hat{p}_\vartheta$.

The eigenvalues $\lambda_n(\vartheta)$ and the corresponding normalized eigenfunctions $U_n(\vartheta;x)$ of the s.a. operator $\hat{p}_\vartheta$ are easily found as the solutions of the eigenvalue problem for the homogeneous first-order differential equation $(\check{p} - \lambda_n(\vartheta))U_n(\vartheta;x) = 0$, where $U_n(\vartheta;x)$ satisfy s.a. boundary condition (6.14), to give

$$\lambda_n(\vartheta) = (2\pi n + \vartheta)/l,\ U_n(\vartheta;x) = (l)^{-1/2}\,\mathrm{e}^{i\lambda_n(\vartheta)x},\quad n \in \mathbb{Z}. \tag{6.15}$$

We show that all other real points u, $u \in \mathbb{R} \setminus \{\lambda_n(\vartheta),\ n \in \mathbb{Z}\}$, are the regular points of $\hat{p}_\vartheta$ and therefore do not belong to its spectrum. By Lemma 2.73, it is sufficient to show that the inhomogeneous first-order differential equation

$$(\check{p} - u)\psi_\vartheta(x,u) = \eta(x),\ \ \forall\eta(x) \in L^2(0,l),$$

has a (unique) solution belonging to D_{p_ϑ} (6.13). It is easy to verify that the required solution is given by

$$\psi_\vartheta(x;u) = i\mathrm{e}^{iux}\left[\mathrm{e}^{i(\vartheta-ul)} - 1\right]^{-1}\left[\mathrm{e}^{i(\vartheta-ul)}\int_0^x \mathrm{d}y\mathrm{e}^{-iuy}\eta(y) + \int_x^l \mathrm{d}y\mathrm{e}^{-iuy}\eta(y)\right].$$

We thus obtain that the spectrum of the s.a. operator $\hat{p}_\vartheta$ is a simple pure discrete spectrum, spec $\hat{p}_\vartheta = \{\lambda_n(\vartheta),\ n \in \mathbb{Z}\}$, where the eigenvalues $\lambda_n(\vartheta)$ and the corresponding eigenfunctions $U_n(\vartheta;x)$ are given by (6.15).

We note that the initial symmetric operator $\hat{p}$ and its closure $\overline{\hat{p}}$ have no eigenvalues, while any complex number z is the eigenvalue of their adjoint $\hat{p}^+$.

It is well known from the theory of Fourier series that the orthonormalized system of functions $\{U_n(0;x),\ n \in \mathbb{Z}\}$ is complete in $L^2(0,l)$. It immediately follows that for any ϑ, the system of functions $\{U_n(\vartheta;x),\ n \in \mathbb{Z}\}$ is also complete in $L^2(0,l)$: the two systems are related by the unitary transformation $\hat{U}(\vartheta) = \mathrm{e}^{i\vartheta x/l}$. The well-known Fourier-series expansion formulas written in terms of the functions $U_n(\vartheta;x)$ are just inversion formulas (5.23), with $(a,b) = [0,l]$, $U_n = U_n(\vartheta;x)$, and $U_\lambda = 0$, for the s.a. operator $\hat{p}_\vartheta$.

6.2 Self-adjoint Extensions and Spectral Problem for Free Particle Hamiltonian

To construct an s.a. quantum Hamiltonian for a one-dimensional free nonrelativistic particle, we start with the corresponding differential operation $\check{\mathcal{H}} = -d_x^2$ (4.7), which follows from the formal canonical quantization rule of replacing the momentum p in the classical Hamiltonian $\mathcal{H} = p^2$ by differential operation (4.6). According to our general scheme, we successively construct the initial symmetric operators $\widehat{\mathcal{H}}$, its adjoint $\widehat{\mathcal{H}}^+$, and some other relevant operators associated with $\check{\mathcal{H}}$. All these operators differ by their domains. However, each of them acts on the corresponding domain by the same differential operation $\check{\mathcal{H}}$. That is why we only indicate the domains of these operators in what follows.

The domain of the initial symmetric operator $\widehat{\mathcal{H}}$ is the space $\mathcal{D}(a,b)$, $D_{\mathcal{H}} = \mathcal{D}(a,b)$, in which case the domain of its adjoint $\widehat{\mathcal{H}}^+$is $D^*_{\check{\mathcal{H}}}(a,b)$, $D_{\mathcal{H}^+} = D^*_{\check{\mathcal{H}}}(a,b)$, the natural domain for $\check{\mathcal{H}}$, as follows from the general theory; see Sect. 4.4.

The deficient subspaces $D_\pm$ and deficiency indices of the operator $\widehat{\mathcal{H}}$ are determined by solutions of the differential equations

$$\check{\mathcal{H}}\psi_\pm(x) = -\psi''_\pm(x) = \pm i\kappa^2\psi_\pm(x)\,, \tag{6.16}$$

where $\kappa > 0$ is an arbitrary, but fixed, parameter of dimensionality of inverse length. The respective general solutions of these equations are

$$\begin{aligned}
&\psi_\pm = c_{1,\pm}\psi_{1,\pm}(x) + c_{2,\pm}\psi_{2,\pm}(x),\ \ \psi_{j,-}(x) = \overline{\psi_{j,+}(x)},\ j = 1,2,\\
&\psi_{1,+}(x) = \exp\left[\frac{(1-i)}{\sqrt{2}}\kappa x\right],\ \ \psi_{2,+}(x) = \exp\left[-\frac{(1-i)}{\sqrt{2}}\kappa x\right],
\end{aligned} \tag{6.17}$$

where $c_{j,\pm}$ are some constants.

From this point on, our considerations depend on the type of interval. We first consider the whole real axis.

6.2.1 *Whole Real Axis*

6.2.1.1 Self-adjoint Hamiltonian

In the case under consideration, the Hilbert space of states is $L^2(\mathbb{R})$. The domain of the initial symmetric operator $\widehat{\mathcal{H}}$ is $D_{\mathcal{H}} = \mathcal{D}(\mathbb{R})$, while the domain of its adjoint $\hat{p}^+$ is $D_{\mathcal{H}^+} = D^*_{\check{\mathcal{H}}}(\mathbb{R})$.

It is evident that both solutions (6.17) and their arbitrary linear combinations are not square-integrable on $\mathbb{R}$ for any κ, which means that deficient subspaces are trivial and both deficiency indices of $\widehat{\mathcal{H}}$ are zero, which implies that the operator $\widehat{\mathcal{H}}$ is essentially s.a., its unique s.a. extension $\widehat{\mathcal{H}}_{\mathfrak{e}}$, $\widehat{\mathcal{H}}_{\mathfrak{e}} = \widehat{\mathcal{H}}^+_{\mathfrak{e}}$, is its closure coinciding with its adjoint, $\widehat{\mathcal{H}}_{\mathfrak{e}} = \overline{\widehat{\mathcal{H}}} = \widehat{\mathcal{H}}^+$, and $D_{\mathcal{H}_{\mathfrak{e}}} = D^*_{\check{\mathcal{H}}}(\mathbb{R})$.

The same result follows from a consideration of the asymmetry form $\Delta_{\mathcal{H}^+}(\psi_*)$. According to (4.36), (4.37), and (4.15), it is represented in terms of the quadratic boundary forms $[\psi_*, \psi_*](\infty/-\infty) \equiv [\psi_*, \psi_*]_{\mathcal{H}}(\infty/-\infty)$ as

$$\Delta_{p^+}(\psi_*) = [\psi_*, \psi_*](x)|_a^b, \quad [\psi_*, \psi_*](x) = \overline{\psi_*'(x)}\psi_*(x) - \overline{\psi_*(x)}\psi_*'(x).$$

By Lemma 2.14, we have $\psi_*, \psi_*' \overset{|x|\to\infty}{\longrightarrow} 0$, $\forall \psi_* \in D^*_{\check{\mathcal{H}}}(\mathbb{R})$. It follows that the boundary forms are trivial and $\Delta_{\mathcal{H}^+}(\psi_*) \equiv 0$, which implies that the operator $\widehat{\mathcal{H}}^+$ is symmetric and therefore the operator $\widehat{\mathcal{H}}$ is essentially s.a.

Therefore, there exists only one s.a. free Hamiltonian $\widehat{\mathcal{H}}_{\mathfrak{e}}$ on the whole real axis.

We now establish the well-known relation between the s.a. free Hamiltonian $\widehat{\mathcal{H}}_{\mathfrak{e}}$ and the s.a. momentum operator $\hat{p}_{\mathfrak{e}}$ constructed in Sect. 6.1.1. We note that the initial symmetric operators $\widehat{\mathcal{H}}$ and $\hat{p}$ are defined on the same domain, $\mathcal{D}(\mathbb{R})$, and it is evident that $\widehat{\mathcal{H}} = \hat{p}^2$. The operator $\hat{p}$ has a unique s.a. extension $\hat{p}_{\mathfrak{e}} = \overline{\hat{p}}$ defined on the natural domain $D^*_{\check{p}}(\mathbb{R})$. By Theorem 2.84, the operator $\left(\overline{\hat{p}}\right)^2$ is s.a. Its restriction to $\mathcal{D}(\mathbb{R})$ coincides with $\hat{p}^2 = \widehat{\mathcal{H}}$, i.e., the operator $\left(\overline{\hat{p}}\right)^2$ is an s.a. extension of $\widehat{\mathcal{H}}$. But $\widehat{\mathcal{H}}_{\mathfrak{e}}$ is a unique s.a. extension of $\widehat{\mathcal{H}}$. This implies that for the whole real axis, the relation[2]

$$\widehat{\mathcal{H}}_{\mathfrak{e}} = \hat{p}_{\mathfrak{e}}^2 = \left(\overline{\hat{p}}\right)^2 \tag{6.18}$$

holds. This relation can be proved independently: it is evident that both operators are associated with the s.a. differential operation $\check{\mathcal{H}} = -d_x^2 = \check{p}^2$, and it is easy to verify that by definition of the operator $\hat{p}_{\mathfrak{e}}^2$, its domain coincides with $D^*_{\check{\mathcal{H}}}(\mathbb{R})$.

[2]This relation is considered evident in most physics textbooks and sometimes incorrectly extended to other intervals; we discuss this point below.

6.2.1.2 Spectrum and Inversion Formulas

In solving the spectral problem, we follow the way described in Sect. 5.3. Following Sect. 5.3.1, in particular, see (5.8), for the special fundamental system of solutions of the homogeneous equation

$$(\check{\mathcal{H}} - W)u(x) = 0, \tag{6.19}$$

we choose the functions

$$u_1(x; W) = \cos(\beta x),\ u_2(x; W) = \beta^{-1}\sin(\beta x),\ \beta = \sqrt{W}, \tag{6.20}$$

normalized at the point $c = 0$ by $u_j^{(k-1)}(0; W) = \delta_{jk},\ j, k = 1, 2$, and evidently real entire in W.

Following Sect. 5.3.4, we evaluate the Green's function of the operator $\widehat{\mathcal{H}}_{\mathfrak{e}}$, finding a unique solution of the inhomogeneous equation

$$(\check{\mathcal{H}} - W)\xi(x) = \eta(x),\ \forall\eta \in L^2(\mathbb{R}),\ \operatorname{Im} W > 0, \tag{6.21}$$

belonging to $D_{\mathcal{H}_{\mathfrak{e}}} = D^*_{\check{\mathcal{H}}}(\mathbb{R})$ and representing it in integral form (5.13) (with the substitution W for z). For W with $\operatorname{Im} W > 0$, we use the parameterization $W = |W|\mathrm{e}^{2i\varphi},\ 0 < \varphi < \pi/2$. Then $\beta = \sqrt{W} = \sqrt{|W|}(\cos\varphi + i\sin\varphi)$, $\operatorname{Im}\beta > 0$, and real W are always denoted by E. The general solution of (6.21) is of the form

$$\xi(x) = c_1\mathrm{e}^{-i\beta x} + c_2\mathrm{e}^{i\beta x} \\ + \frac{i}{2\beta}\left[\int_x^{\infty}\mathrm{e}^{-i\beta(x-y)}\eta(y)\mathrm{d}y + \int_{-\infty}^{x}\mathrm{e}^{i\beta(x-y)}\eta(y)\mathrm{d}y\right]. \tag{6.22}$$

Because $\operatorname{Im}\beta > 0$, the sum of the first two terms on the right-hand side of (6.22) grows exponentially at infinity unless $c_{1,2} = 0$, while by the Cauchy–Schwarz inequality, the integral terms are bounded at the whole axis, which implies that the required solution is given by (6.22) with $c_{1,2} = 0$. It follows that the Green's function is given by

$$G(x, y; W) = \frac{i}{2\beta}\begin{cases}\mathrm{e}^{i\beta(x-y)}, & x > y, \\ \mathrm{e}^{-i\beta(x-y)}, & x < y.\end{cases}$$

Following Sect. 5.3.2, we calculate the matrix $M_{jk}(0; W)$, see (5.15) (with the substitution W for z and taking into account that in our case, the quasiderivatives coincide with ordinary derivatives),

$$M_{jk}(0; W) = \frac{i}{2\beta}\begin{pmatrix}1 & -i\beta \\ i\beta & \beta^2\end{pmatrix} = \frac{1}{2}i\beta^{2j-3}\delta_{jk} + i\sigma^2_{jk},$$

and then the derivative $\sigma'_{jk}(E)$ of the matrix spectral function, see (5.19) (with the substitution E for λ),

$$\sigma'_{jk}(E) = \pi^{-1} \operatorname{Im} M_{jk}(0; E + i0) = \frac{1}{2\pi} \operatorname{Im}[i\beta^{2j-3}]\big|_{\beta=\sqrt{E+i0}} \delta_{jk}.$$

In calculating the derivative of the matrix spectral function, we have to distinguish the semiaxis $E \geq 0$ and $E < 0$:

(a) For $E \geq 0$, we have $\beta = \sqrt{E + i0} = \sqrt{E}$, and we obtain

$$\sigma'_{jk}(E) = \frac{1}{2\pi} \left(\sqrt{E}\right)^{2j-3} \delta_{jk}. \tag{6.23}$$

(b) For $E < 0$, we have $\beta = \sqrt{E + i0} = i\sqrt{|E|}$, and we obtain

$$\sigma'_{jk}(E) = 0. \tag{6.24}$$

According to Sect. 5.3.3, the spectrum of the operator $\widehat{\mathcal{H}}_{\mathfrak{e}}$ consists of the growth points of the matrix spectral function. It then follows from (6.23) and (6.24) that $\operatorname{spec} \widehat{\mathcal{H}}_{\mathfrak{e}} = \mathbb{R}_+$. Because the matrix $\sigma'_{jl}(E)$ is nonsingular, the spectrum of $\widehat{\mathcal{H}}_{\mathfrak{e}}$ is twofold (twofold degenerate).

And finally, the general inversion formulas (5.20) (with the substitutions E for λ and Φ for φ) in our particular case in which $n = 2$, $\rho_{jk}(E) = \frac{1}{2\pi}(\sqrt{E})^{2j-3}\delta_{jk}$, and $\varkappa_{jk,m} = 0$ become

$$\eta(x) = \frac{1}{2\pi} \int_0^\infty \left[\Phi_1(E) \frac{\cos\left(\sqrt{E}x\right)}{\sqrt{E}} + \Phi_2(E) \sin(\sqrt{E}x) \right] \mathrm{d}E,$$

$$\Phi_1(E) = \int_{-\infty}^\infty \cos\left(\sqrt{E}x\right) \eta(x)\mathrm{d}x\,,\; \Phi_2(E) = \int_{-\infty}^\infty \frac{\sin\left(\sqrt{E}x\right)}{\sqrt{E}} \eta(x)\mathrm{d}x.$$

After the natural change of the variable E to $p = \sqrt{E}$ and the replacement of the functions $\Phi_{1,2}(E)$ by the functions $\phi_{1,2}(p)$ given by

$$\phi_1(p) = (\pi)^{-1/2} \Phi_1(E),\; \phi_2(p) = (\pi)^{-1/2} p\Phi_2(E),$$

the inversion formulas are reduced to the conventional sine–cosine form of the Fourier transformation,

$$\eta(x) = (\pi)^{-1/2} \int_0^\infty [\phi_1(p)\cos(px) + \phi_2(p)\sin(px)]\,\mathrm{d}p,$$

$$\phi_1(p) = (\pi)^{-1/2} \int_{-\infty}^\infty \cos(px)\psi(x)\mathrm{d}x\,,\; \phi_2(p) = (\pi)^{-1/2} \int_{-\infty}^\infty \sin(px)\psi(x)\mathrm{d}x.$$

The following remark is worth noting.

The eigenfunctions $\cos\left(\sqrt{E}x\right)$ and $\sin\left(\sqrt{E}x\right)/\sqrt{E}$ respectively are even and odd under the transformation $x \to -x$, or equivalently, they are symmetric or antisymmetric with respect to the origin. This is a consequence of a diagonal structure of the spectral matrix $\sigma'_{jk}(E)$ (6.23). In turn, the latter is a manifestation of the fact that that the unitary parity operator $\hat{P}$ defined by $\hat{P}\psi(x) = \psi(-x)$ commutes with the operator $\widehat{\mathcal{H}}_{\mathfrak{e}}$. As a consequence, the Hilbert space $L^2(\mathbb{R})$ is decomposed into the orthogonal direct sum of the two subspaces $L^2_{(+)}(\mathbb{R})$ and $L^2_{(-)}(\mathbb{R})$ of the respective symmetric and antisymmetric functions that are the eigenspaces of $\hat{P}$ with the respective eigenvalues $+1$ and -1, $L^2(\mathbb{R}) = L^2_{(+)}(\mathbb{R}) \dot{\oplus} L^2_{(-)}(\mathbb{R})$. The subspaces $L^2_{(+)}(\mathbb{R})$ and $L^2_{(-)}(\mathbb{R})$ reduce the operator $\widehat{\mathcal{H}}_{\mathfrak{e}}$, so that the inversion formulas for $\widehat{\mathcal{H}}_{\mathfrak{e}}$ in the whole space $L^2(\mathbb{R})$ actually split into a couple of independent inversion formulas in the subspaces $L^2_{(+)}(\mathbb{R})$ and $L^2_{(-)}(\mathbb{R})$.

In conclusion, we note that all the results in this section directly follow from the representation (6.18); in particular, the eigenfunctions of $\widehat{\mathcal{H}}_{\mathfrak{e}}$ are certain linear combinations of the eigenfunctions of $\hat{p}_{\mathfrak{e}}$.

6.2.2 A Semiaxis

6.2.2.1 Self-adjoint Hamiltonians

The Hilbert space of states is $L^2(\mathbb{R}_+)$. The domains of the initial symmetric operator $\widehat{\mathcal{H}}$ and its adjoint $\widehat{\mathcal{H}}^+$ are respectively $D_{\mathcal{H}} = \mathcal{D}(\mathbb{R}_+)$ and $D_{\mathcal{H}^+} = D^*_{\check{\mathcal{H}}}(\mathbb{R}_+)$.

The deficient subspaces $D_\pm$ as the spaces of square-integrable solutions (6.17) of equations (6.16) are easily evaluated. It suffices to find D_+, and then D_- is obtained by complex conjugation. Among the two linearly independent solutions $\psi_{1,+}(x)$ and $\psi_{2,+}(x)$, only $\psi_{2,+}(x)$ is square-integrable on the semiaxis. This means that the deficiency indices in our case are $m_\pm = 1$, and we have a one-parameter $U(1)$ family $\{\widehat{\mathcal{H}}_U\}$ of s.a. extensions of the initial symmetric operator $\widehat{\mathcal{H}}$. If we parameterize elements U of the group $U(1)$ by the angle θ: $U = e^{i\theta}$, $\theta \in \mathbb{S}(-\pi, \pi)$, then each s.a. extension is naturally labeled by an angle θ, $\widehat{\mathcal{H}}_U = \widehat{\mathcal{H}}_\theta$. A specification of s.a. operators $\widehat{\mathcal{H}}_\theta$, which are associated with $\check{\mathcal{H}}$, by s.a. boundary conditions is performed in accordance with Theorem 4.17: $\check{\mathcal{H}}$ is an even s.a. differential operator of second order, $n = 2$, on an interval $(a, b) = (0, \infty)$, the left endpoint $a = 0$ is regular, the right endpoint $b = \infty$ is singular, and the right boundary form is equal to zero by Lemma 2.14. For illustration, we trace the specification in detail. The normalized basis functions in $D_\pm$ are respectively $e_\pm = \sqrt[4]{2\kappa^2}\psi_{2,\pm}(x)$, a unique basis function $e_U \equiv e_\theta$ in the one-dimensional subspace $(\hat{I}+\hat{U})D_{+}\subset D_{\mathcal{H}_{\theta}}$ is $e_{\theta}=e_{+}+\mathrm{e}^{i\theta}e_{-}$, the matrix $E_{1/2,U}(a)$ in (4.80) defined by (4.78) is a column given by[3]

$$E_{1/2,\theta}(0)=\sqrt[4]{2\kappa^{2}}\begin{pmatrix}1+\mathrm{e}^{i\theta}\\ 2^{-1/2}\kappa\left[(i-1)-(1+i)\,\mathrm{e}^{i\theta}\right]\end{pmatrix},$$

the matrix $\mathcal{E}$ (4.66) is given by $\mathcal{E}=\operatorname{antdiag}(1,-1)$, the column $\Psi_{U}(a)$ (4.68) is given by

$$\Psi_{\theta}(0)=\begin{pmatrix}\psi_{\theta}(0)\\ \psi_{\theta}'(0)\end{pmatrix},$$

so that s.a. boundary conditions (4.79) specifying $\widehat{\mathcal{H}}_{\theta}$ become

$$\left(1+\mathrm{e}^{-i\theta}\right)\psi_{\theta}'(0)+2^{-1/2}\kappa\left[(1+i)+(1-i)\,\mathrm{e}^{-i\theta}\right]\psi_{\theta}(0)=0\,,$$

or equivalently

$$\psi_{\theta}'(0)\cos\nu=\kappa\psi_{\theta}(0)\sin\nu,\quad\tan\nu=2^{-1/2}(\tan\theta/2-1)\,. \tag{6.25}$$

As θ ranges from $-\pi$ to π, ν ranges from $-\pi/2$ to $\pi/2$, and $\nu=\pm\pi/2$ ($\theta=\pm\pi$) equivalently yield the s.a. boundary condition $\psi(0)=0$. It is natural to change the notation $\widehat{\mathcal{H}}_{\theta}\to\widehat{\mathcal{H}}_{\nu}$ and $\psi_{\theta}\to\psi_{\nu}$. In this notation, the boundary condition (6.25) becomes

$$\psi_{\nu}'(0)\cos\nu=\kappa\psi_{\nu}(0)\sin\nu,\ \ \nu\in\mathbb{S}(-\pi/2,\pi/2)\,. \tag{6.26}$$

So, for a free particle on a semiaxis, there exists a family $\{\widehat{\mathcal{H}}_{\nu}\}$ of s.a. operators associated with the differential operation $\check{\mathcal{H}}$; their domains $D_{\mathcal{H}_{\nu}}$ are given by

$$D_{\mathcal{H}_{\nu}}=\left\{\psi_{\nu}:\psi_{\nu}\in D_{\check{\mathcal{H}}}^{*}(\mathbb{R}_{+})\,;\ \psi_{\nu}\text{ satisfies }(6.26)\right\}.$$

Each of the operators $\widehat{\mathcal{H}}_{\nu}$ is a candidate for the s.a. Hamiltonian for a free particle on the semiaxis. In physics, the boundary condition (6.26) with $\nu=\pm\pi/2$ is conventional. In particular, it is characteristic for a free radial motion in the s-wave. However, the boundary condition (6.26) with $|\nu|<\pi/2$ is also encountered.

We note that even though the Hamiltonian with a fixed ν depends on the parameter κ, the whole family $\{\widehat{\mathcal{H}}_{\nu}\}$ is the same for any choice of κ. We also emphasize that if $\nu\neq\pm\pi/2$, the dimensional parameter κ, which is lacking in the initial differential operation $\check{\mathcal{H}}$, enters QT as an additional parameter specifying a Hamiltonian.

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[3] We note in passing that the correctness of the calculation, which is very simple in this case, is confirmed by the fact that both necessary conditions $\operatorname{rank}E_{1/2,\theta}=1$ and $E_{1/2,\theta}^{+}(0)\,\mathcal{E}E_{1/2,\theta}(0)=0$ hold; see the remark following Theorem 4.17.

The same results are easily obtained by the asymmetry form method without evaluating the deficient subspaces. According to the above-mentioned properties of $\mathcal{H}$, our case falls within the realms of the cases considered at the end of Sect. 4.7 and associated with formulas (4.133) and (4.134). In our case, the columns $\Psi_{U,\tau+}(a)$ and $\Psi_{\tau-}(a)$ defined by (4.130) and (4.131) are the respective numbers

$$\psi_{U,\tau+}(0) \equiv \psi_{\nu,\tau+}(0) = \psi_\nu(0) + i\tau\psi'_\nu(0),$$
$$\psi_{\nu,\tau-}(0) = \psi_\nu(0) - i\tau\psi'_\nu(0),$$

where the unitary matrix $U \in U(1)$ is a complex number of unit modulus. If we set $\tau = 1/\kappa$ and $U = \mathrm{e}^{2i\nu}$, $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, s.a. boundary conditions (4.134) directly reduce to (6.26).

We recall that for a particle on a semiaxis, no s.a. momentum operator exists, but there exist two closed densely defined operators $\hat{g}_1$ and $\hat{g}_2$ associated with $\check{p}$, namely, $\hat{g}_1 = \hat{g}_2^+ = \overline{p}$ and $\hat{g}_2 = \hat{g}_1^+ = \hat{p}^+$; see Sect. 6.1.2.

Then, according to Theorem 2.84, the operators $\widehat{\mathcal{H}}_{(1)} = \hat{p}^+\overline{p}$ and $\widehat{\mathcal{H}}_{(2)} = \overline{p}\hat{p}^+$ are s.a. operators associated with $\check{\mathcal{H}}$. We first evaluate the domain $D_{\mathcal{H}_{(1)}}$ of the operator $\widehat{\mathcal{H}}_{(1)}$ following from its definition. A function ψ belonging to $D_{\mathcal{H}_{(1)}}$ must belong to $D_{\overline{p}}$ given by (6.10); its derivative ψ' belonging to $R_{\overline{p}}$ must be a.c. for to belong to D_{p^+}; and its second derivative ψ'' must be square-integrable. All this means that $\psi \in D^*_{\check{\mathcal{H}}}(\mathbb{R}_+)$. On the other hand, by Lemma 2.14, the requirement $\psi \in D^*_{\check{\mathcal{H}}}(\mathbb{R}_+)$ implies that ψ' is square-integrable. It follows that

$$D_{\mathcal{H}_{(1)}} = \{\psi : \psi \in D^*_{\check{\mathcal{H}}}(\mathbb{R}_+),\ \psi(0) = 0\},$$

i.e., $D_{\mathcal{H}_{(1)}} = D_{\mathcal{H}_{\pm\pi/2}}$, and therefore $\widehat{\mathcal{H}}_{(1)} = \widehat{\mathcal{H}}_{\pm\pi/2}$. Similarly we obtain that

$$D_{\mathcal{H}_{(2)}} = \{\psi :\ \psi \in D^*_{\check{\mathcal{H}}}(\mathbb{R}_+),\ \psi'(0) = 0\},$$

i.e., $D_{\mathcal{H}_{(2)}} = D_{\mathcal{H}_0}$, and therefore $\widehat{\mathcal{H}}_{(2)} = \widehat{\mathcal{H}}_0$.

The general problem of representations of all the Hamiltonians $\widehat{\mathcal{H}}_\nu$ as quadratic combinations of first-order differential momentum-like operators (we call such representations the oscillator representations) is considered in [77].

6.2.2.2 Spectrum and Inversion Formulas

We begin by following a method adopted in Sect. 6.2.1. For the special fundamental system $u_j(x; W)$, $j = 1, 2$, of solutions of the homogeneous equation (6.19) on the semiaxis, we take the same functions (6.20) reduced to the semiaxis.

Next is an evaluation of the Green's function of the operator $\widehat{\mathcal{H}}_\nu$ by finding a unique solution of the inhomogeneous equation (6.21) on the semiaxis belonging to $D_{\mathcal{H}_\nu}$. The general solution of this equation can be represented as

$$\xi(x) = c_1 \mathrm{e}^{-i\beta x} + c_2 \mathrm{e}^{i\beta x} + \frac{i}{2\beta}\left[\mathrm{e}^{-i\beta x}\int_x^\infty \mathrm{e}^{i\beta y}\eta(y)\mathrm{d}y + \mathrm{e}^{i\beta x}\int_0^x \mathrm{e}^{-i\beta y}\eta(y)\mathrm{d}y\right],$$

where $c_{1,2}$ are some constants. Using the Cauchy–Schwarz inequality, it is easy to verify that the last three summands on the right-hand side of this representation are bounded as $x \to \infty$, while the first one grows exponentially unless $c_1 = 0$. The condition $\xi \in D_{\mathcal{H}_\nu}$ implies that ξ is square-integrable and satisfies s.a. boundary condition (6.26). The first requirement fixes the constant c_1, $c_1 = 0$, while the second requirement fixes the constant c_2,

$$c_2 = -\frac{i}{2}(\kappa \sin\nu + i\beta\cos\nu)[\beta(\kappa\sin\nu - i\beta\cos\nu)]^{-1}\int_0^\infty \mathrm{e}^{i\beta x}\eta(x)\mathrm{d}x\,,$$

so that the required solution is

$$\begin{aligned}\xi(x) &= (\kappa\sin\nu - i\beta\cos\nu)^{-1}\\ &\quad\times\left[\mathrm{e}^{i\beta x}\int_0^x u_\nu(y;W)\eta(y)\mathrm{d}y + u_\nu(x;W)\int_x^\infty \mathrm{e}^{i\beta y}\eta(y)\mathrm{d}y\right],\\ u_\nu(x;W) &= \cos(\beta x)\cos\nu + \kappa\frac{\sin(\beta x)}{\beta}\sin\nu.\end{aligned}$$

It follows that the Green's function of the operator $\widehat{\mathcal{H}}_\nu$ is given by

$$G(x,y;W) = (\kappa\sin\nu - i\beta\cos\nu)^{-1}\begin{cases}\mathrm{e}^{i\beta x}u_\nu(y;W), & x > y,\\ u_\nu(x;W)\mathrm{e}^{i\beta y}, & x < y.\end{cases}$$

We note that the function $u_\nu(x;W)$ is a solution of the homogeneous equation (6.19), which is real entire in W and satisfies s.a. boundary condition (6.26).

The matrix $M_{jk}(0;W)$ calculated in accordance with (5.15) and its imaginary part respectively are

$$\begin{aligned}M_{jk}(0) &= (\kappa\sin\nu - i\beta\cos\nu)^{-1}\begin{pmatrix}\cos\nu & \kappa\sin\nu\\ i\beta\cos\nu & i\beta\kappa\sin\nu\end{pmatrix},\\ \operatorname{Im} M_{jk}(0;W) &= \operatorname{Im} A_\nu(W)(\mathbf{n}\otimes\mathbf{n})_{jk}, \quad \mathbf{n} = \{n_j\} = (\cos\nu, \kappa\sin\nu),\\ A_\nu(W) &= [\cos\nu(\kappa\sin\nu - i\beta\cos\nu)]^{-1}.\end{aligned}$$

We could next calculate the derivative $\sigma'_{jk}(E)$ of the matrix spectral function in accordance with (5.19), find the spectrum of the operator $\widehat{\mathcal{H}}_\nu$, and explicitly write the inversion formulas (5.20). On the other hand, the structure of the matrix Im M_{jk} indicates that the functions u_1 and u_2 enter the inversion formulas not independently but as a unique linear combination $n_1u_1 + n_2u_2 = u_\nu$. This observation shows that the spectrum of the operator $\widehat{\mathcal{H}}_\nu$ is actually simple. We prove this fact using the simple guiding functional method.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_\nu(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{\mathcal{H}_\nu}.$$

It is easy to see that this functional belongs to the class E of simple guiding functionals considered in Sect. 5.4.1 with the functions $U(x, W) = u_\nu(x, W)$ and $\tilde{U}(x) = \tilde{u}_\nu(x; \lambda_0)$, where

$$\tilde{u}_\nu(x; W) = -\cos(\beta x)\sin\nu + \kappa\beta^{-1}\sin(\beta x)\cos\nu$$

is a solution of the homogeneous equation (6.19), which is linearly independent of $u_\nu(x, W)$ and real entire in W. Therefore, the spectrum of $\widehat{\mathcal{H}}_\nu$ is simple.

We rewrite the Green's function as

$$\begin{aligned} G(x, y; W) = {} & \Omega(W)u_\nu(x; W)u_\nu(y; W) \\ & - \kappa^{-1}\begin{cases} \tilde{u}_\nu(x; W)u_\nu(y; W), & x > y, \\ u_\nu(x; W)\tilde{u}_\nu(y; W), & x < y, \end{cases} \end{aligned}$$

where

$$\Omega(W) = \kappa^{-1}\frac{\kappa\cos\nu + i\beta\sin\nu}{\kappa\sin\nu - i\beta\cos\nu}.$$

Using this representation and representations (5.22) and (5.21) with λ changed to E, we obtain that the derivative of the spectral function is given by $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega(E + i0)$. We consider the semiaxis $E \geq 0$ and $E < 0$ separately.

(1) For $E \geq 0$, we have $\beta = \sqrt{E + i0} = \sqrt{E}$, the function $\Omega(E + i0) = \Omega(E)$ is a finite complex function, and we obtain

$$\sigma'(E) = \sqrt{E}\left[\pi(\kappa^2\sin^2\nu + E\cos^2\nu)\right]^{-1}.$$

(2) For $E < 0$, we have $\beta = \sqrt{E + i0} = i\sqrt{|E|}$, and formally,

$$\Omega(E) = \frac{\kappa\cos\nu - \sqrt{|E|}\sin\nu}{\kappa\sin\nu + \sqrt{|E|}\cos\nu} = \omega^{-1}(E),$$

but we have to distinguish two regions of the extension parameter ν:

(a) For $0 \leq \nu < \pi/2$ and $\nu = \pm\pi/2$, the function $\omega(E)$ is a real function without zeros, so that $\mathrm{Im}\,\Omega(E + i0) = \mathrm{Im}\,\Omega(E)$, $\forall E < 0$, and we obtain $\sigma'(E) = 0$.

(b) For $-\pi/2 < \nu < 0$, the function $\omega(E)$ is a real function with a single simple zero at the point $E = \tau_\nu = -\kappa^2\tan^2\nu$,

$$\mathrm{Im}\,\omega(E) = 0,\ \forall E < 0;\ \omega(E) \neq 0,\ E \neq \tau_\nu;\ \omega(\tau_\nu) = 0,\ \tau_\nu = -\kappa^2\tan^2\nu,$$

and using Lemma 5.17, we obtain

$$\sigma'(E) = 2\kappa \cos^{-2}\nu \tan|\nu|\delta(E - \tau_\nu),$$

which means that in this case, there exists a negative energy level $\tau_\nu = -(\kappa \tan \nu)^2$.

The final results for the spectrum and eigenfunctions of the operators $\widehat{\mathcal{H}}_\nu$ are as follows.

For $0 \le \nu < \pi/2$ and $\nu = \pm\pi/2$, the spectrum of the operator $\widehat{\mathcal{H}}_\nu$ is simple and continuous, spec $\widehat{\mathcal{H}}_\nu = \mathbb{R}_+$, and its corresponding generalized eigenfunctions $U_E^{(\nu)}(x)$ forming a complete orthonormalized system in $L^2(\mathbb{R}_+)$ are

$$U_E^{(\nu)}(x) = \sqrt{\frac{\sqrt{E}}{\pi(\kappa^2 \sin^2\nu + E\cos^2\nu)}}\, u_\nu(x; E),\ \ E \ge 0. \tag{6.27}$$

For $-\pi/2 < \nu < 0$, the spectrum of the operator $\widehat{\mathcal{H}}_\nu$ is simple, contains a continuous nonnegative part and a point part consisting of a unique negative energy level τ_ν,

$$\operatorname{spec}\widehat{\mathcal{H}}_\nu = \mathbb{R}_+ \cup \left\{\tau_\nu = -(\kappa \tan\nu)^2\right\},$$

and the corresponding eigenfunctions forming a complete orthonormalized system in $L^2(\mathbb{R}_+)$ are the generalized eigenfunctions of the continuous spectrum $U_E^{(\nu)}(x)$ given by the same formula (6.27), but of course with different ν, and a unique eigenfunction

$$U^{(\nu)}(x) = \cos^{-1}\nu\sqrt{2\kappa\tan|\nu|}\,u(x; \tau_\nu)$$

of the point spectrum.

The inversion formulas for $\nu = \pm\pi/2$ written in terms of the functions $U_E(x) = \sqrt{2/\pi}\sin\left(\sqrt{E}x\right)$ coincide with the standard sine decomposition on the semiaxis; the cosine decomposition on the semiaxis is covered by the inversion formulas with $\nu = 0$.

6.2.3 A Finite Interval

6.2.3.1 Self-adjoint Hamiltonians

The Hilbert space of states is $L^2(0, l)$. The domains of the initial symmetric operator $\widehat{\mathcal{H}}$ and its adjoint $\widehat{\mathcal{H}}^+$ are respectively $D_{\mathcal{H}} = \mathcal{D}(0, l)$ and $D_{\mathcal{H}^+} = D^*_{\check{\mathcal{H}}}(0, l)$. The point is that $\check{\mathcal{H}}$ is a regular even, second-order, s.a. differential operation.

A construction of all s.a. extensions of $\widehat{\mathcal{H}}$, in particular their specification by s.a. boundary conditions, was already given above by three different methods in

Sect. 4.5, see (4.61) or (4.62), in Sect. 4.6, see (4.65) or (4.69), and (implicitly) in Sect. 4.7, see (4.132), as an illustration of Theorems 4.12, 4.15, and 4.24, respectively.

In our opinion, the most direct and convenient specification of s.a. extensions $\widehat{\mathcal{H}}_U$ of $\widehat{\mathcal{H}}$ in terms of s.a. boundary conditions is due to the asymmetry form method as applied to regular even s.a. differential operations, which is presented in Sect. 4.7 and associated with formulas (4.127), (4.128), (4.129), (4.130), (4.131), and (4.132). For a dimensional parameter τ, we take the length l of the interval, and lest the notation be overloaded, we omit the index l. With this convention, s.a. boundary conditions (4.132) in our case become

$$\begin{pmatrix} \psi(l) - il\psi'(l) \\ \psi(0) + il\psi'(0) \end{pmatrix} = U \begin{pmatrix} \psi(l) + il\psi'(l) \\ \psi(0) - il\psi'(0) \end{pmatrix}, \tag{6.28}$$

where $U \in U(2)$.

The whole $U(2)$ family $\{\widehat{\mathcal{H}}_U,\ U \in U(2)\}$ of s.a. operators associated with $\check{\mathcal{H}}$ is completely determined by their domains $D_{\mathcal{H}_U}$ given by

$$D_{\mathcal{H}_U} = \left\{\psi : \psi \in D^*_{\check{\mathcal{H}}}(0,l) \ \text{and satisfy (6.28)}\right\}. \tag{6.29}$$

Each $\widehat{\mathcal{H}}_U$ can be considered a candidate for a Hamiltonian for a free particle on a finite interval.

In the spectral analysis of free Hamiltonians on a finite interval, we restrict ourselves to the two well-known Hamiltonians, the Hamiltonian $\widehat{\mathcal{H}}_{-I}$ corresponding to the choice $U = -I$,

$$D_{\mathcal{H}_{-I}} = \{\psi : \psi \in D^*_{\check{\mathcal{H}}}(0,l),\ \psi(0) = \psi(l) = 0\}, \tag{6.30}$$

and the Hamiltonian $\widehat{\mathcal{H}}_{\sigma^1}$ corresponding to the choice $U = \sigma^1$,

$$D_{\mathcal{H}_{\sigma^1}} = \{\psi : \psi \in D^*_{\check{\mathcal{H}}}(0,l),\ \psi(l) = \psi(0),\ \psi'(l) = \psi'(0)\}. \tag{6.31}$$

In physics, the zero s.a. boundary conditions in (6.30) are conventionally associated with a particle in an infinite rectangular potential well, whereas the periodic s.a. boundary conditions in (6.31) are conventionally associated with a particle on a circle (a rigid rotator) or with an ideal gas in a box.

We note that the Hamiltonian $\widehat{\mathcal{H}}_{-I}$ allows the representation $\widehat{\mathcal{H}}_{-I} = \hat{p}^+\overline{\hat{p}}$, where the operators $\overline{\hat{p}}$ and $\hat{p}^+$ are defined in Sect. 6.1.3.

For the Hamiltonian $\widehat{\mathcal{H}}_{\sigma^1}$, the representation

$$\widehat{\mathcal{H}}_{\sigma^1} = \hat{p}_0^2 \tag{6.32}$$

holds, where the operator $\hat{p}_0$ is one of the family $\{\hat{p}_\vartheta\}$ of the momentum operators on the interval $[0,l]$ with $\vartheta = 0$; see Sect. 6.1.3. These representations (6.32) are easily verified following the definition of the right-hand sides. By the way, the representation (6.32) suggests a way to construct some of the possible free Hamiltonians. Namely, the one-parameter family $\{\hat{p}_\vartheta\}$ of s.a. momentum operators generates the one-parameter family $\{\widehat{\mathcal{H}}_\vartheta\}$ of s.a. operators defined by

$$\widehat{\mathcal{H}}_\vartheta = \hat{p}_\vartheta^2. \tag{6.33}$$

As directly follows from their definition, these operators are associated with the differential operation $\check{\mathcal{H}}$, and their domains are given by

$$D_{\mathcal{H}_\vartheta} = \{\psi : \psi \in D^*_{\check{\mathcal{H}}}(0,l)\,,\ \psi(l) = \mathrm{e}^{i\vartheta}\psi(0),\ \psi'(l) = \mathrm{e}^{i\vartheta}\psi'(0)\}. \tag{6.34}$$

The one-parameter family $\{\widehat{\mathcal{H}}_\vartheta\}$ is a subfamily of the whole four-parameter family $\{\widehat{\mathcal{H}}_U\}$ of free Hamiltonians that is obtained if we take the subfamily $\{U_\vartheta\}$ of 2×2 unitary matrices, where $U_\vartheta = \operatorname{antidiag}\left(\mathrm{e}^{-i\vartheta}, \mathrm{e}^{i\vartheta}\right)$ in (6.28).

6.2.3.2 Spectrum and Inversion Formulas

In both cases labeled below by I and II, for the special fundamental system $u_j(x;W)$, $j = 1,2$, of solutions of homogeneous equation (6.19) on the interval $[0,l]$, we take the same functions (6.20) reduced to the interval.

(I) We first consider the s.a. operator $\widehat{\mathcal{H}}_{-I}$. The simple guiding functional method proves to be applicable to this operator.

Because the function u_2 satisfies the s.a. boundary condition in (6.30) for the operator $\widehat{\mathcal{H}}_{-I}$ at the left endpoint, $u_2(0,W) = 0$, we consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x u_2(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{\mathcal{H}_{-I}}.$$

It is easy to verify that this functional belongs to the class E of simple guiding functionals considered in Sect. 5.4.1 with the functions $U = u_2$ and $\tilde{U} = u_1$, whence it follows that the spectrum of the operator $\widehat{\mathcal{H}}_{-I}$ is simple and the derivative of its spectral function is evaluated using representations (5.22) and (5.21) (with λ changed to E).

Next is an evaluation of the Green's function $G(x,y;W)$ of the operator $\widehat{\mathcal{H}}_{-I}$ by the standard procedure.

The general solution of the inhomogeneous equation (6.21) on the interval $[0,l]$ can be represented as

$$\xi(x) = c_1 u_1(x;W) + c_2 u_2(x;W) + u_2(x;W) \\ \times \int_x^l u_1(y;W)\eta(y)\mathrm{d}y + u_1(x;W)\int_0^x u_2(y;W)\eta(y)\mathrm{d}y, \tag{6.35}$$

where $c_{1,2}$ are some constants. The requirement that $\xi(x) \in D_{\mathcal{H}_{-I}}$ is equivalent to the requirement that $\xi(x)$ satisfies the boundary conditions $\xi(0) = \xi(l) = 0$, which fixes the constants c_1 and c_2, namely,

$$c_1 = 0, \; c_2 = \beta^{-1} \cot \beta l \int_0^l u_2(y; W)\eta(y)\mathrm{d}y.$$

It follows that the Green's function is given by

$$\begin{aligned} G(x, y; W) &= \omega^{-1}(W)u_2(x; W)u_2(y; W) \\ &\quad + \begin{cases} u_1(x; W)u_2(y; W), & x > y, \\ u_2(x; W)u_1(y; W), & x < y, \end{cases} \quad \omega(W) = -\beta^{-1}\tan(\beta l), \end{aligned} \tag{6.36}$$

and according to (5.22), with $u = u_2$, $c = 0$, and λ changed to E, the derivative $\sigma'(E)$ of the spectral function is given by

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \omega^{-1}(E + i0).$$

Because the function $\omega(E + i0) = \omega(E)$ is real-valued, the derivative $\sigma'(E)$ differs from zero only at the zeros of $\omega(E)$.

We have to distinguish the semiaxis $E < 0$ and $E \geq 0$.

For $E < 0$, we have $\beta = \sqrt{E + i0} = i\sqrt{|E|}$, the real-valued function $\omega(E)$ has no zeros,

$$\omega(E) = \overline{\omega(E)} = -\left(\sqrt{|E|}\right)^{-1} \tan h \left(l\sqrt{|E|}\right) \neq 0, \; \forall E < 0,$$

and we obtain $\sigma'(E) = 0$.

For $E \geq 0$, we have $\beta = \sqrt{E + i0} = \sqrt{E} \geq 0$, the real-valued function $\omega(E)$ has an infinite sequence $\{E_n = \pi^2 n^2 l^{-2}\}_1^\infty$ of simple zeros going to infinity,

$$\omega(E_n) = -\beta_n^{-1} \tan(\beta_n l) = 0, \; \beta_n = \pi n l^{-1},$$

$$\omega'(E_n) = -\frac{l^3}{2\pi^2 n^2}, \; n \in \mathbb{N},$$

and using Lemma 5.17, we obtain

$$\sigma'(E) = \sum_{n \in \mathbb{N}} 2\pi^2 n^2 l^{-3} \delta\left(E - E_n\right),$$

so that E_n are the eigenvalues of $\widehat{\mathcal{H}}_{-I}$ and the corresponding eigenfunctions are $u_2(x; E_n)$.

The conclusion is that the spectrum of the operator $\widehat{\mathcal{H}}_{-I}$ is simple and pure point,

$$\operatorname{spec} \widehat{\mathcal{H}}_{-I} = \left\{E_n = \pi^2 n^2 l^{-2}, \; n \in \mathbb{N}\right\},$$

and the normalized eigenfunctions

$$U_n(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{\pi n}{l} x\right), \quad n \in \mathbb{N}, \tag{6.37}$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

We note that the eigenfunctions (6.37) are even if n is odd, and odd if n is even, under the transformation $x \to l - x$, or equivalently, they are symmetric or antisymmetric with respect to the point $x = l/2$, which is in agreement with the fact that the unitary parity operator $\hat{P}$ defined by $\hat{P}\psi(x) = \psi(l - x)$ commutes with $\widehat{\mathcal{H}}_{-I}$. An extended comment on this point would be an appropriately modified copy of the remark on the relation between the operator $\widehat{\mathcal{H}}_{\mathfrak{c}}$ and the parity operator $\hat{P}$ on the whole axis; see the end of Sect. 6.2.1.

(II) Passing to the s.a. operator $\widehat{\mathcal{H}}_{\sigma^1}$, we note that because the s.a. boundary conditions for $\widehat{\mathcal{H}}_{\sigma^1}$, see (6.31), are nonsplit, the simple guiding functional method is not applicable, and in the spectral analysis of this operator, we have to deal with the generic matrix spectral function and formulas (5.15), (5.19), and (5.20), completely similarly to the analysis in Sect. 6.2.1.2.

We begin with the Green's function. The general solution of inhomogeneous equation (6.21) on the interval $[0, l]$ is given by the same (6.35). The requirement that $\xi(x) \in D_{\mathcal{H}_{\sigma^1}}$ is equivalent to the requirement that $\xi(x)$ satisfies the periodic boundary conditions $\xi(0) = \xi(l)$ and $\xi'(0) = \xi'(l)$, which fixes the constants c_1 and c_2, namely,

$$c_1 = -\frac{1}{2}\int_0^l \left[\beta^{-1}\cot(\beta l/2)u_1(y;W)\eta(y)\mathrm{d}y + u_2(y;W)\right]\eta(y)\mathrm{d}y,$$

$$c_2 = -\frac{1}{2}\int_0^l \left[u_1(y;W) + \beta\cot(\beta l/2)u_2(y;W)\right]\eta(y)\mathrm{d}y.$$

It follows that the Green's function $G(x, y; W)$ of the operator $\widehat{\mathcal{H}}_{\sigma^1}$ is given by

$$G(x, y; W) = -(2\beta)^{-1}\left\{\sin(\beta|x - y|) + \cot(\beta l/2)\cos[\beta(x - y)]\right\}. \tag{6.38}$$

The matrix $M_{jk}(0, W)$ given by (5.15) with $c = 0$, and the substitution $z \to W$ is

$$M_{jk}(0, W) = \omega_j^{-1}(W)\delta_{jk} + \frac{i}{2}\left(\sigma^2\right)_{jk}, \; \omega_j(W) = -2\beta^{3-2j}\tan(\beta l/2),$$

and accordingly, the derivative $\sigma'_{jk}(E)$ of the matrix spectral function defined by (5.19) is given by

$$\sigma'_{jk}(E) = \pi^{-1}\,\mathrm{Im}\,\omega_j^{-1}(E + i0)\,\delta_{jk}.$$

Because the functions $\omega_j(E + i0) = \omega_j(E)$, $j = 1, 2$, are real-valued, the derivative $\sigma'_{jk}(E)$ differs from zero only at the zeros of the functions $\omega_j(E)$.

We have to distinguish the semiaxis $E < 0$ and $E \geq 0$.

For $E < 0$, we have $\beta = \sqrt{E + i0} = i\sqrt{|E|}$, the real-valued functions $\omega_j(E)$ has no zeros,

$$\omega_j(E) = \overline{\omega_j(E)} = -2\left(\sqrt{|E|}\right)^{3-2j} \tan h\left(\frac{1}{2} l \sqrt{|E|}\right) \neq 0,\ \forall E < 0,$$

and we obtain $\sigma'_{jk}(E) = 0$.

For $E \geq 0$, we have $\beta = \sqrt{E + i0} = \sqrt{E}$, the real-valued functions $\omega_1(E)$ and $\omega_2(E)$ have the respective infinite sequences $\{E_n = 4\pi^2 n^2 l^{-2}\}_0^\infty$ and $\{E_n\}_1^\infty$ of simple zeros going to infinity,

$$\omega_1(E_n) = -2\beta_n \tan(\beta_n l/2) = 0,\ \beta_n = \frac{2\pi n}{l},\ n \in \mathbb{Z}_+,$$
$$\omega_1'(0) = -l,\ \omega_1'(E_n) = -l/2,\ n \in \mathbb{N};$$
$$\omega_2(E_n) = -2\beta_n^{-1} \tan(\beta_n l/2) = 0,\ \omega_2'(E_n) = -\frac{l^3}{8\pi^2 n^2},\ n \in \mathbb{N},$$

and using Lemma 5.17, we obtain

$$\sigma_{11}'(E) = l^{-1}\delta(E) + 2\sum_{n\in\mathbb{N}} l^{-1}\delta(E - E_n),$$
$$\sigma_{22}'(E) = \sum_{n\in\mathbb{N}} 8\pi^2 n^2 l^{-3}\delta(E - E_n),\ \sigma_{ij}(E) = 0,\ i \neq j,$$

so that E_n, $n \in \mathbb{Z}_+$, are the eigenvalues of $\widehat{\mathcal{H}}_{\sigma^1}$ and the corresponding eigenfunctions are $u_1(x; E_n)$, $n \in \mathbb{Z}_+$, and $u_2(x; E_n)$, $n \in \mathbb{N}$.

The conclusion is that the spectrum of the operator $\widehat{\mathcal{H}}_{\sigma^1}$ is pure point,

$$\operatorname{spec} \widehat{\mathcal{H}}_{\sigma^1} = \left\{E_n = 4\pi^2 n^2 l^{-2},\ n \in \mathbb{Z}_+\right\},$$

and twofold degenerate, except the ground level $E_0 = 0$, and the normalized eigenfunctions

$$U_n(x) = \sqrt{\frac{2}{l}} \cos\left(\frac{2\pi n}{l} x\right),\ n \in \mathbb{Z}_+,$$
$$V_n(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{2\pi n}{l} x\right),\ n \in \mathbb{N}, \tag{6.39}$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

The inversion formulas (5.20) written in terms of the normalized eigenfunctions (6.39) become

$$\eta(x) = \sum_{k\in\mathbb{Z}_+} a_k U_k(x) + \sum_{n\in\mathbb{N}} b_n V_n(x),$$

$$a_k = \int_0^l U_k(x)\eta(x)\mathrm{d}x,\ b_n = \int_0^l V_n(x)\eta(x)\mathrm{d}x.$$

The functions $U_n(x)$ are even, while the functions $V_n(x)$ are odd under the transformation $x \to l - x$. The structure of the matrix spectral function is such that the inversion formulas actually are split into a couple of independent inversion formulas in the subspaces $L^2_{(+)}(0,l)$ and $L^2_{(-)}(0,l)$ of the respective even and odd functions that reduce the Hamiltonian $\widehat{\mathcal{H}}_{\sigma^1}$. Completely similarly to the comment on the operator $\widehat{\mathcal{H}}_{-I}$ at the end of the part I above, an extended comment on this point would be an appropriately modified copy of the remark on the relation between the operator $\widehat{\mathcal{H}}_{\mathfrak{e}}$ and the parity operator $\hat{P}$ on the whole axis at the end of Sect. 6.2.1.

It should be noted that all the results of the spectral analysis of the Hamiltonian $\widehat{\mathcal{H}}_{\sigma^1}$ directly follow from the representation (6.32); in particular, the eigenfunctions of $\widehat{\mathcal{H}}_{\sigma^1}$ are certain linear combinations of the eigenfunctions of $\hat{p}_0$.

To conclude this section, we note that all the results concerning both Hamiltonians $\widehat{\mathcal{H}}_{-I}$ and $\widehat{\mathcal{H}}_{\sigma^1}$, well known to physicists, can be easily obtained by the conventional method adopted in physical textbooks if supplemented with a certain argument. The eigenvalues and eigenfunctions of both operators are easily evaluated. It remains only to show that all the points E of the real energy axis not coinciding with the eigenvalues are regular ones, so that the spectra of the operators are pure point. But this follows from the existence of the Green's functions $G(x, y; E)$ at such points; see (6.36) and (6.38) respectively.

6.3 Explanation of Paradoxes

In this section, it is convenient to restore the Planck constant $\hbar$ and the factor $(2m)^{-1}$ in front of the free particle Hamiltonian.

6.3.1 *Paradox 1*

We recall that the first paradox presented in Sect. 1.3.1 is a consequence of the relation

$$\left(\psi_p, [\hat{x}, \hat{p}]\psi_p\right) = \left(\psi_p, \hat{x}\hat{p}\psi_p\right) - \left(\psi_p, \hat{p}\hat{x}\psi_p\right) = 0, \tag{6.40}$$

where $\hat{p}$ is an s.a. momentum operator, and $\psi_p(x)$ is an eigenvector of this operator. Obviously, canonical commutation relations (1.4) and uncertainty principle (1.7) are necessarily violated if (6.40) holds.

In the following, we resolve the paradox based on the results obtained in this chapter. We consider separately three cases: the whole real axis, a semiaxis, and a finite interval.

Consider a particle on the whole real axis $\mathbb{R}$ with the Hilbert space $L^2(\mathbb{R})$. As was demonstrated in Sect. 6.1.1, in this case, there exists a unique s.a. momentum operator $\hat{p}_{\mathfrak{e}}$. But this operator has no eigenfunctions, i.e., ψ_p in (6.40) do not exist as vectors in $L^2(\mathbb{R})$: solutions $\varphi = \mathrm{e}^{ipx}$ of the differential equations $\check{p}\varphi(x) = p\varphi(x)$ are not square-integrable on the whole axis.

Consider a particle on the semiaxis $\mathbb{R}_+$ with the Hilbert space of states $L^2(\mathbb{R}_+)$. As was demonstrated in Sect. 6.1.2, in this case, there is no s.a. momentum operator at all, and therefore, eigenvectors ψ_p in (6.40) are meaningless.

We thus obtain that in the cases of the whole axis and a semiaxis, the matrix elements in (6.40), and therefore (6.40) itself, make no sense.

Consider a particle on an interval $[0, l]$ with the Hilbert space of states $L^2(0, l)$. As was demonstrated in Sect. 6.1.3, in this case, there exists a family $\{\hat{p}_\vartheta, \vartheta \in \mathbb{S}\,(0, 2\pi)\}$ of s.a. momentum operators. Their domains D_{p_ϑ} are given by (6.13), and in particular, the functions belonging to D_{p_ϑ} must satisfy the boundary condition

$$\psi_\vartheta\,(l) = \mathrm{e}^{i\vartheta}\psi_\vartheta\,(0)\,, \tag{6.41}$$

and their spectra are pure point spectra. The eigenvalues $\lambda_n(\vartheta)$ and eigenfunctions $\psi_{\vartheta n}(x)$ of the operator $\hat{p}_\vartheta$, $\hat{p}_\vartheta\psi_{\vartheta n} = \lambda_n(\vartheta)\psi_{\vartheta n}$, are presented in (6.15). The functions $\psi_{\vartheta n}$ certainly satisfy condition (6.41). We now turn to the matrix element on the left-hand side of (6.40), where ψ_p is identified with $\psi_{\vartheta n}$. The first term $(\psi_{\vartheta n}, \hat{x}\hat{p}_\vartheta\psi_{\vartheta n})$ is evidently equal to $\lambda_n(\vartheta)\,(\psi_{\vartheta n}, \hat{x}\psi_{\vartheta n})$. But as for the second term $(\psi_{\vartheta n}, \hat{p}_\vartheta\hat{x}\psi_{\vartheta n})$, we cannot write the equality

$$(\psi_{\vartheta n}, \hat{p}_\vartheta\hat{x}\psi_{\vartheta n}) = (\hat{p}_\vartheta\psi_{\vartheta n}, \hat{x}\psi_{\vartheta n}) = \lambda_n(\vartheta)\,(\psi_{\vartheta n}, \hat{x}\psi_{\vartheta n})$$

to provide zero on the right-hand side of (6.40). The reason is that the vector $\hat{x}\psi_{\vartheta n}$ does not belong to the domain D_{p_ϑ}, because the function $x\psi_{\vartheta n}(x)$ does not satisfy condition (6.41): the operator $\hat{x}$ removes the vector $\psi_{\vartheta n}$ from the domain D_{p_ϑ}. The equality $(\psi_{\vartheta n}, \hat{p}_\vartheta\hat{x}\psi_{\vartheta n}) = (\hat{p}_\vartheta\psi_{\vartheta n}, \hat{x}\psi_{\vartheta n})$ is meaningless, because the matrix element $(\psi_{\vartheta n}, \hat{p}_\vartheta\hat{x}\psi_{\vartheta n})$ is not defined.

Because Heisenberg uncertainty relation (1.7) is derived by considering matrix elements of the operator $[\hat{x}, \hat{p}]$, a similar consideration makes it possible to explain the second part of the first paradox related to the Heisenberg uncertainty relation.

6.3.2 Paradox 2

We recall that the second paradox presented in Sect. 1.3.2 is a consequence of the assertion that the Hamiltonian for a nonrelativistic particle in an infinite rectangular potential well, which we call a free particle on a finite interval, can be represented as $\widehat{\mathcal{H}} = \hat{p}^2/2m$, and therefore, it commutes with the s.a. momentum operator $\hat{p}$. If so, both operators must have a common set of eigenfunctions, which is not the case.

An explanation of this paradox is based on the results obtained in Sects. 6.1.3 and 6.2.3, where it was demonstrated that there exists only one s.a. Hamiltonian for a particle in an infinite rectangular potential well. It was denoted by $\widehat{\mathcal{H}}_{-I}$, and its domain is given by (6.30). On the other hand, as was just mentioned in Sect. 6.3.1, there exists the one-parameter family $\{\hat{p}_\vartheta\}$ of s.a. momentum operators on a finite interval. This family generates the one-parameter family $\{\widehat{\mathcal{H}}_\vartheta = (\hat{p}_\vartheta)^2/2m\}$ of s.a. Hamiltonians; see (6.33) (where the factor $1/2m$ is omitted). However, none of these Hamiltonians coincides with $\widehat{\mathcal{H}}_{-I}$. Indeed, none of the domains $D_{\mathcal{H}_\vartheta}$ given by (6.34) coincides with $D_{\mathcal{H}_{-I}}$. Moreover, the eigenfunctions of any $\hat{p}_\vartheta$ given by (6.15) do not belong to the domain of $\widehat{\mathcal{H}}_{-I}$, and the eigenfunctions of $\widehat{\mathcal{H}}_{-I}$ given by (6.37) do not belong to the domain of any $\hat{p}_\vartheta$. The operators $\widehat{\mathcal{H}}_{-I}$ and $\hat{p}_\vartheta$ do not commute and have no common eigenfunctions. This is consistent with the physical fact that the particle momentum changes (is not conserved) due to the reflection from the wall.

An example in which we do not encounter such a paradox offers a free particle on a circle. The s.a. Hamiltonian $\widehat{\mathcal{H}}_{\sigma^1}$ for such a particle is defined by (6.31) and allows the representation $\widehat{\mathcal{H}}_{\sigma^1} = (\hat{p}_0)^2/2m$, where $\hat{p}_0$ is the s.a. momentum operator $\hat{p}_\vartheta|_{\vartheta=0}$; see (6.32) (where the factor $1/2m$ is omitted). The operators $\widehat{\mathcal{H}}_{\sigma^1}$ and $\hat{p}_0$ have a common set of eigenfunctions. The paradox is also absent in the case of a free particle on the whole axis, which was considered in Sects. 6.1.1 and 6.2.1, where it was demonstrated that there exist a unique s.a. Hamiltonian $\widehat{\mathcal{H}}_\mathfrak{e}$ and a unique s.a. momentum operator $\hat{p}_\mathfrak{e}$ for such a particle and the representation $\widehat{\mathcal{H}}_\mathfrak{e} = \hat{p}_\mathfrak{e}^2/2m$ holds; see (6.18). It is easy to verify that both operators act on their domains as $\check{\mathcal{H}}\check{p}$. This means that the operators $\widehat{\mathcal{H}}_\mathfrak{e}$ and $\hat{p}_\mathfrak{e}$ commute, which agrees with physical considerations. In addition, both operators have a common complete system of generalized eigenfunctions $\exp(ikx)$, $k \in \mathbb{R}$.

6.3.3 Paradox 3

The third paradox described in Sect. 1.3.3 treats an s.a. momentum operator $\hat{p}$ for a particle on a finite interval $[0, l]$ and the matrix elements $p_{mn} = (e_m, \hat{p}e_n)$ of the operator with respect to the orthonormal basis $\{e_n\}_1^\infty$ (1.10). It turns out that contrary to naïve expectation, the matrix p_{mn} is not Hermitian; see (1.11). The incorrect assumption underlying the paradox is that basis (1.10) belongs to the domain of an s.a. momentum operator for a particle on a finite interval. But the functions belonging to the domains D_{p_ϑ} of the admissible momentum operators $\hat{p}_\vartheta$ must satisfy boundary conditions (6.41), $\psi(l) = \mathrm{e}^{i\vartheta}\psi(0)$, whereas for the functions $e_n(x)$, we have

$$e_n(l) = (-1)^n e_n(0). \tag{6.42}$$

It is easy to see that there is no angle ϑ, one and the same for all n, so that condition (6.42) could be identified with condition (6.41). This means that there is no domain D_{p_ϑ} such that the basis $\{e_n\}_1^\infty$ as a whole belongs to D_{p_ϑ}. For any ϑ, some elements of the basis $\{e_n\}_1^\infty$ do not belong to the domain of the s.a. operator $\hat{p}_\vartheta$, so that the matrix elements p_{mn} and p_{nm} in (1.11) are not defined for any m and n, and therefore, inequality (1.11) itself makes no sense.

6.3.4 Paradox 4

The fourth paradox described in Sect. 1.3.4 treats the case of a free particle in an infinite rectangular potential well on an interval $[0, l]$ with an s.a. Hamiltonian $\widehat{\mathcal{H}}$ for which the paradoxical inequality

$$\left(\psi, \left(\widehat{\mathcal{H}}\right)^2 \psi\right) \neq \left(\widehat{\mathcal{H}}\psi, \widehat{\mathcal{H}}\psi\right) \tag{6.43}$$

with a particular state ψ given by (1.12), $\psi(x) = Nx(x-l)$, N a normalization factor, seemingly holds.

An explanation of this paradox is as follows. As was already said above in Sect. 6.3.2, a unique Hamiltonian for a particle in an infinite rectangular potential well is $\widehat{\mathcal{H}}_{-I}$. The functions belonging to its domain $D_{\mathcal{H}_{-I}}$ satisfy the boundary conditions $\psi(0) = \psi(l) = 0$. It is easy to see that the state ψ belongs to $D_{\mathcal{H}_{-I}}$, but the state $\widehat{\mathcal{H}}_{-1}\psi$, $\widehat{\mathcal{H}}_{-1}\psi(x) = \text{const} \neq 0$, just does not belong to $D_{\mathcal{H}_{-I}}$, the state $\left(\widehat{\mathcal{H}}_{-I}\right)^2 \psi$ is not defined, and therefore, inequality (6.43) makes no sense.

6.3.5 Paradox 5

The fifth paradox described in Sect. 1.3.5 is concerned with a solution (1.15) of the Schrödinger equation (1.13) for a free particle on a finite interval $[0, l]$. The right-hand side in (1.13) is treated as $\widehat{\mathcal{H}}\psi(t, x)$, under a special choice (1.14) of the initial state. The presented solution vanishes with time, which means that the evolution is not unitary; the particle "disappears" with time evolution. It was stated in advance that the origin of the paradox is an intolerable choice of the initial state: initial wave function (1.14) does not belong to the domain of any admissible s.a. Hamiltonian, which is irreconcilable with the Schrödinger equation. We now are able to prove this statement. As was demonstrated in Sect. 6.2.3, there exists a $U(2)$ family $\{\widehat{\mathcal{H}}_U\}$ of s.a. Hamiltonians for a free particle on the finite interval; their domains $D_{\mathcal{H}_U}$ are given by (6.29). We can directly verify that the initial state ψ_0 presented by the wave function $\psi_0(x) = \psi(0, x)$ (1.14) belongs to none of the domains $D_{\mathcal{H}_U}$, $\psi_0 \notin D_{\mathcal{H}_U}$, $\forall U$, i.e., does not satisfy s.a. boundary conditions (6.28) with any 2×2

unitary matrix U (of course, ψ in (6.28) has to be changed to ψ_0). The proof is by contradiction. Let $\psi_0(x)$ satisfy boundary conditions (6.28) with some U, which implies that the two two-component vectors

$$\Psi_{0+} = \begin{pmatrix} \psi(l) + il\psi'(l) \\ \psi(0) - il\psi'(0) \end{pmatrix}, \; \Psi_{0-} = \begin{pmatrix} \psi(l) - il\psi'(l) \\ \psi(0) + il\psi'(0) \end{pmatrix},$$

belonging to $\mathbb{C}^2$ have the same norm, $\Psi_{0-}^+\Psi_{0-} - \Psi_{0+}^+\Psi_{0+} = 0$, because the matrix U is unitary. But a simple calculation yields $\Psi_{0-}^+\Psi_{0-} - \Psi_{0+}^+\Psi_{0+} = 4|C|^2\varkappa(e^{2\varkappa} - 1) \neq 0$ because $\varkappa = kl/\sqrt{2}\hbar \neq 0$, which is a contradiction. As a consequence, the "solution" $\psi(t,x)$ (1.15) of the Schrödinger equation also belongs to none of $D_{\mathcal{H}_U}$, $\psi(t) \notin D_{\mathcal{H}_U}$. This means that the state $\widehat{\mathcal{H}}_U\psi(t)$, the right-hand side of the Schrödinger equation, is not defined, and therefore, the Schrödinger equation with the initial state ψ_0 and the solution $\psi(t)$ makes no sense. An extended comment on this point is given below.

6.3.6 Some Remarks to Paradox 5

In considering the fifth paradox, we encounter an evolving state that formally is a solution of the Schrödinger equation with a given initial state, but the norm of the evolving state is not conserved with time, which implies the nonunitarity of evolution. We would like to make a comment on this point.

In QM, we actually have two ways for determining the time evolution of a system with an s.a. Hamiltonian $\hat{H}$. The first one consists in solving the Cauchy problem for the Schrödinger equation (1.3) with given initial data. This way is not universal. It requires that the initial state and the evolving state belong to the domain D_H of the Hamiltonian. In cases in which the Schrödinger equation has the form of partial differential equations, this requirement means that a solution of the Cauchy problem is sought under certain boundary conditions specifying the s.a. Hamiltonian; otherwise, a solution of the Cauchy problem is not unique. The second way consists in evaluating the unitary evolution operator

$$\hat{U}(t) = \exp\left\{-\frac{i}{\hbar}\hat{H}t\right\},$$

and then applying it to the initial state. This way is universal, it is applicable to any initial state ψ because the operator $\hat{U}(t)$ is bounded and defined everywhere, the evolving state

$$\psi(t) = \hat{U}(t)\psi \tag{6.44}$$

$\psi(t) = \hat{U}(t)\psi$ always exists, and the time evolution is unitary. As an illustration, let ψ_n be a complete orthonormalized system of eigenvectors of $\hat{H}$, and let an initial state be ψ. The initial state can be represented as $\psi = \sum_n a_n \psi_n$, $a_n = (\psi_n, \psi)$, $\|\psi\|^2 = \sum_n |a_n|^2$. Then the evolving state $\psi_U(t)$ is given by

$$\psi(t) = \hat{U}(t)\psi = \sum a_n e^{-iE_n t/\hbar} \psi_n; \tag{6.45}$$

it is evidently defined at any instant of time and its norm is evidently conserved with time, $\|\psi(t)\| = \|\psi\|$.

The unitary evolution operator $\hat{U}(t)$ determines an integral evolution law (6.44), which is universal, whereas the Schrödinger equation (1.3) determines a differential evolution law, which is not universal. The Schrödinger equation is conventionally derived by an integral evolution law (6.44) by differentiating the latter with respect to time t. But the derivative $i\hbar d_t \hat{U}(t)\psi = \hat{H}\hat{U}(t)\psi$ exists iff the initial state ψ, and then also the evolving state $\psi(t) = \hat{U}(t)\psi$, belongs to D_H, in other words, the derivative $i\hbar d_t \hat{U}(t)$ of the evolution operator exists and is equal to $\hat{H}\hat{U}(t)$ only on the domain D_H of the Hamiltonian $\hat{H}$. Applied to the above example, this means that if $\psi = \sum a_n \psi_n$, then there must be $\|\hat{H}\psi\|^2 = \|\hat{H}\psi(t)\|^2 = \sum_n E_n^2 |a_n| < \infty$ for $\psi(t)$ (6.45) to satisfy the Schrödinger equation.

Turning back to the fifth paradox, we now can say that we can construct an evolving wave function $\psi(t, x)$ with the initial wave function $\psi_0(x)$ (1.14) for any admissible s.a. Hamiltonian $\widehat{\mathcal{H}}_U$ using formula (6.45). But this function does not satisfy the Schrödinger equation with the given $\widehat{\mathcal{H}}_U$ because $\psi_0(x)$ does not belong to any D_{H_U}. It also does not coincide with function (1.15) that is the solution of differential equation (1.13) with the initial condition (1.14), but under no additional conditions, and is therefore a nonunique solution of (1.13). To prove the latter assertion, it is sufficient to verify that a function $\widetilde{\psi}(t, x)$ defined on the interval $[0, l]$ by

$$\widetilde{\psi}(t, x) = \frac{1}{\sqrt{t}} \int_b^\infty dy \exp\left[i \frac{m}{2\hbar t}(x - y)^2\right] \varphi(y),$$

where $\varphi(y)$ is a smooth function with compact support on the semiaxis $[b, \infty)$, $b > l$, is a solution of differential equation (1.13) on $[0, l]$ satisfying the initial condition $\widetilde{\psi}(0, x) = 0$ because

$$\lim_{t \to 0} \frac{1}{\sqrt{t}} \exp\left[i \frac{m}{2\hbar t}(x - y)^2\right] \sim \delta(x - y).$$

A conclusion that deserves remembering is that not every state—in particular not every wave function—that evolves unitarily satisfies the Schrödinger equation, but only the one that belongs to the domain of the corresponding s.a. Hamiltonian.

Chapter 7
A One-Dimensional Particle in a Potential Field

In this chapter, we consider s one-dimensional nonrelativistic particle in a potential field.[1] As was already mentioned, see Chap. 4, all possible s.a. quantum Hamiltonians corresponding to such systems are associated with the s.a. differential operation $\check{H}$ given by (4.8),

$$\check{H} = \check{\mathcal{H}} + V(x) = -d_x^2 + V(x)\,,\ V(x) = \overline{V(x)}\,, \tag{7.1}$$

which we call the *Schrödinger differential operation*.

Our aim is to study possible s.a. quantum Hamiltonians associated with $\check{H}$ and the corresponding spectral problems. Such quantum Hamiltonians are sometimes called the *Schrödinger operators*.

We call an equation of the form

$$\left(\check{H} - W\right)\psi(x) = 0,\ x \in (a, b) \subset \mathbb{R}, \tag{7.2}$$

where W is a complex constant, the *one-dimensional (stationary) Schrödinger equation*. If W is real, it is denoted by E. We conventionally call E the energy, $V(x)$ the potential, and $\psi(x)$ the wave function.

[1] In this and subsequent chapters, we set $\hbar = 1$ and omit the factor $1/2m$ in $\check{\mathcal{H}}$.

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7.1 Some Remarks on the Schrödinger Differential Operation

7.1.1 First Remark

In constructing s.a. extensions of symmetric differential operators on an interval (a, b), it is useful to know the corresponding boundary forms $[\psi_*, \psi_*](a/b)$, $\forall \psi_* \in D^*_{\check{H}}(a, b)$; see Chap. 4. Sometimes, this is a difficult task that requires a knowledge of function asymptotics at the interval boundaries. However, it turns out that there may exist simple estimates of the potential $V(x)$ in (7.1) that allow one to make immediate conclusions about the boundary forms without calculating the asymptotics. Below, we present two sufficient conditions for the potential $V(x)$ in the Schrödinger operation on the interval (a, ∞) with $|a| < \infty$ that guarantee that the boundary form will be zero at infinity. In our opinion, these conditions are rather general and at the same time are rather simple from the standpoint of applications.

Theorem 7.1. *Let the Schrödinger differential operation be given on the interval (a, ∞) with $|a| < \infty$. Then the boundary form at infinity is zero, $[\psi_*, \psi_*](\infty) = 0$, $\forall \psi_* \in D^*_{\check{H}}(a, \infty)$, if either*

$$V(x) \in L^2(N, \infty), \; a < N < \infty, \tag{7.3}$$

i.e., the potential $V(x)$ is square-integrable at infinity, or

$$V(x) > -Kx^2, \;\; x > N, \; K > 0, \tag{7.4}$$

i.e., the potential is bounded from below for sufficiently large x by a negative quadratic parabola.[2]

Proof. First we suppose that condition (7.3) takes place. Then the proof of the theorem is based on the observation proved below that under this condition, the function $x^{-1/2}\psi_*'$ is bounded at infinity,

$$\left|x^{-1/2}\psi_*'\right| < C(\psi_*) < \infty, \, x > N, \; \forall \psi_* \in D^*_{\check{H}}(a, \infty), \tag{7.5}$$

where $C(\psi_*)$ is a constant that may be different for different ψ_*. It follows that the function $x^{-1/2}\overline{\psi_*}\psi_*'$ is square-integrable at infinity together with ψ_*, and therefore, the function $x^{-1/2}[\psi_*, \psi_*] = x^{-1/2}\left(\overline{\psi_*'}\psi_* - \overline{\psi_*}\psi_*'\right)$ is also square-integrable at infinity. On the other hand, the finiteness of the boundary form $[\psi_*, \psi_*](\infty)$,

$$[\psi_*, \psi_*] \to C_1(\psi_*), \; x \to \infty, \; |C_1(\psi_*)| < \infty, \tag{7.6}$$

[2]The condition (7.3) was first mentioned in [127], and the condition (7.4) in [90]. The latter condition is a particular case of a more general condition [106, 116].

implies that $x^{-1/2}[\psi_*, \psi_*] \to x^{-1/2}C_1(\psi_*)$ as $x \to \infty$. But the function at the left is square-integrable at infinity, whereas the limit function at the right is not square-integrable unless $C_1(\psi_*)$ is equal to zero. This proves that $[\psi_*, \psi_*](\infty) = C_1(\psi_*) = 0$. It remains to prove estimate (7.5). For this purpose, we recall that $\psi_* \in D^*_{\check{H}}(a, \infty)$ means that ψ_* and $\varphi = \check{H}\psi_*$ belong to $L^2(a, \infty)$, and therefore $\psi_*, \varphi \in L^2(N, \infty)$. For any $\eta \in L^2(N, \infty)$, the function $\int_N^x \mathrm{d}y\, |\eta|^2$ is bounded,

$$\int_N^x \mathrm{d}y\, |\eta|^2 < C_2(\eta) < \infty. \tag{7.7}$$

In particular,

$$\int_N^x \mathrm{d}y\, |\psi_*|^2 < C_2(\psi_*), \ \int_N^x \mathrm{d}y\, |\varphi|^2 < C_2(\varphi).$$

Using the Cauchy–Schwarz inequality, we obtain

$$\left|\int_N^x \mathrm{d}y\varphi\right| < C_2^{1/2}(\varphi)\sqrt{x-N}, \ x > N. \tag{7.8}$$

On the other hand, if $V \in L^2(N, \infty)$ (as well as ψ_*), then the function $V\psi_*$ is integrable on the interval (N, ∞), and therefore, the function $\int_N^x \mathrm{d}yV\psi_*$ is bounded on the same interval,

$$\left|\int_N^x \mathrm{d}yV\psi_*\right| < C_3(\psi_*) < \infty. \tag{7.9}$$

Integrating $\check{H}\psi_* = \varphi$ on the interval (N, x), we first obtain the equality

$$\psi'_*(x) = \int_N^x \mathrm{d}yV\psi_* - \int_N^x \mathrm{d}y\varphi + \psi'_*(N),$$

and then, using (7.8) and (7.9), we obtain that $\forall \psi_* \in D^*_{\check{H}}(a, \infty)$ the inequality

$$\left|\psi'_*(x)\right| < C_3(\psi_*) + C_2^{1/2}(\varphi)\sqrt{x-N} + \left|\psi'_*(N)\right|, \ x > N,$$

holds, whence follows estimate (7.5), which completes the proof of the theorem under the condition (7.3).

We now turn to condition (7.4). Here the proof of the theorem is based on the observation (proved below) that under this condition, the function $x^{-1}\psi'_*$ is square-integrable at infinity together with ψ_*,

$$\int_N^\infty \mathrm{d}y\left|y^{-1}\psi'_*\right|^2 < C_4(\psi_*) < \infty, \ \forall \psi_* \in D^*_{\check{H}}(a, \infty). \tag{7.10}$$

It follows that the function $x^{-1}\overline{\psi_*}\psi_*'$ is also integrable at infinity, and therefore, the function $x^{-1}[\psi_*, \psi_*]$ is integrable at infinity as well. On the other hand, the finiteness of the boundary form $[\psi_*, \psi_*](\infty)$, see (7.6), implies that $x^{-1}[\psi_*, \psi_*] \to C_1(\psi_*)\, x^{-1}$ as $x \to \infty$. But the function $x^{-1}[\psi_*, \psi_*]$ is integrable at infinity, whereas the limit function $C_1(\psi_*)\, x^{-1}$ is not integrable unless $C_1(\psi_*) = 0$. This proves that $[\psi_*, \psi_*](\infty) = C_1(\psi_*) = 0$. It remains to prove the validity of formula (7.10). This is proved by contradiction. We first make some preliminary estimates based on the condition that the functions ψ_* and $\varphi = \check{H}\psi_*$ belong to $L^2(a, \infty)$. It follows from this condition that (see (7.7)) that

$$\int_N^x \mathrm{d}y \left|y^{-3}\psi_*\right|^2 < C_6(\psi_*) < \infty, \ \int_N^x \mathrm{d}y \left|y^{-4}\psi_*\right|^2 < C_7(\psi_*) < \infty,$$
$$\left|\int_a^x \mathrm{d}y y^{-2}\left(\overline{\varphi}\psi_* + \overline{\psi_*}\varphi\right)\right| < 2\sqrt{C_2(\varphi)\, C_7(\psi_*)}. \tag{7.11}$$

Condition (7.4) implies that $x^{-2}V(x) > -K$, $K > 0$, for $x > N$ and therefore,

$$\int_N^x \mathrm{d}y y^{-2} V |\psi_*|^2 > -K \int_N^x \mathrm{d}y\, |\psi_*|^2 > -KC_2(\psi_*)\,. \tag{7.12}$$

On the other hand, we have the equality

$$\overline{\psi_*}\varphi + \psi_*\overline{\varphi} = -d_x^2 |\varphi|^2 + 2\left|\psi_*'\right|^2 + 2V|\psi_*|^2.$$

Multiplying both sides by x^{-2} and integrating, we obtain the equality

$$x^{-2}d_x|\psi_*(x)|^2 = 2\int_N^x \mathrm{d}y \left|y^{-1}\psi_*'\right|^2 + 2\int_N^x \mathrm{d}y y^{-2}V|\psi_*|^2$$
$$-6\int_N^x \mathrm{d}y y^{-4}|\psi_*|^2 - \int_N^x \mathrm{d}y \left(\overline{\chi_*}\psi_* + \overline{\psi_*}\chi_*\right) - 2x^{-3}|\psi_*(x)|^2 + C_8(\psi_*)\,,$$
$$C_8(\psi_*) = \left(x^{-2}d_x|\psi_*|^2 + 2x^{-3}|\psi_*|^2\right)\Big|_{x=N}.$$

Taking estimates (7.11) and (7.12) into account, we arrive at the inequality

$$d_x|\psi_*|^2 > x^2\left[2I - C_9(\psi_*)\right] - 2x^{-3}|\psi_*|^2, \ \ I = \int_N^x \mathrm{d}y \left|y^{-1}\psi_*'\right|^2,$$
$$C_9 = 2KC_2(\psi_*) + 6C_7(\psi_*) + 2\sqrt{C_2(\chi_*)\, C_7(\psi_*)} - C_8(\psi_*)\,.$$

Suppose now that the integral I diverges as $x \to \infty$. Then for sufficiently large x, $x > c > N$, the estimate $2I - C_9(\psi_*) > C_{10}(\psi_*) > 0$ holds, and we arrive at the inequality

$$d_x|\psi_*|^2 > x^2 C_{10}(\psi_*) - 2x^{-3}|\psi_*|^2\,.$$

Integrating this inequality and taking estimates (7.11) into account, we obtain

$$|\psi_*|^2 > C_{10}(\psi_*)\,x^3/3 - 2C_6(\psi_*) - C_{10}(\psi_*)\,c^3/3 + |\psi_*(c)|^2,$$

whence it follows that $|\psi_*|^2 \to \infty$ as $x \to \infty$, which contradicts the square-integrability of the function ψ_* at infinity. This contradiction proves that the function $x^{-1}\psi_*'$ is square-integrable at infinity, i.e., (7.10) holds, which completes the proof of the theorem under the condition (7.4).

The above criteria can clearly be extended to the Schrödinger differential operation defined on the interval $(-\infty, b)$, or on the whole real axis $\mathbb{R}$, providing the triviality of the boundary forms at the infinite endpoints:

Theorem 7.2. *Suppose the Schrödinger differential operation is given on the interval $(-\infty, b)$ with $|b| < \infty$. Then the boundary form at infinity is zero, $[\psi_*, \psi_*](-\infty) = 0$, $\forall \psi_* \in D^*_{\check{H}}(-\infty, b)$, if either*

$$V(x) \in L^2(-\infty, -N), \tag{7.13}$$

where N is a finite real number, or

$$V(x) > -Kx^2, \; x < -N, \;\; K > 0. \tag{7.14}$$

Suppose the Schrödinger differential operation is given on the interval R. Then the boundary forms at infinity are zero, $[\psi_*, \psi_*](\pm\infty) = 0$, $\forall \psi_* \in D^*_{\check{H}}(\mathbb{R})$, if $V(x)$ satisfies either condition (7.3), or (7.4) on ∞, and either condition (7.13), or (7.14) on $-\infty$.

7.1.2 Second Remark

Consider the Schrödinger differential operation defined on (a, b) with a a regular endpoint and b singular. We recall that the condition that a is a regular endpoint means that the potential $V(x)$ is integrable at the left endpoint,[3] i.e., is integrable on any interval (a, c), $c < b$. We know, see Chap. 4, (4.48), that in such a case, the deficiency indices of the initial symmetric Schrödinger operator $\hat{H}$ can be either $m_\pm = 1$ or $m_\pm = 2$. Self-adjoint boundary conditions have the simplest form when $m_\pm = 1$. As follows from Lemma 4.16, in such a case, the boundary form vanishes on the singular endpoint b, and s.a. boundary conditions have the form $\psi'(0) = \lambda\psi(0)$ according to Theorem 4.22. Self-adjoint Schrödinger operators $\widehat{\mathcal{H}}_\lambda$ of a free

[3] We recall that we consider only such potentials that are locally integrable inside the interval (a, b). We also recall that for us, integrability always means absolute integrability.

particle on the semiaxis associated with the differential operation $\check{\mathcal{H}} = \check{H}\big|_{V=0}$ can serve as an illustration of the latter fact; see Sect. 6.2. An inverse statement holds as well: if the boundary form vanishes on the singular endpoint b, then the deficiency indices are $m_\pm = 1$; see Sect. 4.7.

Therefore, the initial symmetric Schrödinger operator $\hat{H}$ on the interval (a, ∞), $|a| < \infty$, with a potential $V(x)$ that obeys either condition (7.3) or (7.4) has the deficiency indices $m_\pm = 1$.

At this point, we refer also to a useful result concerning the maximum deficiency indices $m_\pm = n$ of the initial symmetric operator $\hat{f}$ associated with an even s.a. differential operation $\check{f}$ of order n defined on the interval with one regular and one singular endpoint. It turns out (see [9, 116]) that the maximality of the deficiency indices is uniquely related to the maximality of the dimension of the kernel of the adjoint operator, $\dim\ker \hat{f}^+$, i.e., of the number of linearly independent square-integrable solutions of the homogeneous equation $(\check{f} - W)u = 0$ of order n. Namely, the initial symmetric operator $\hat{f}$ has the maximum deficiency indices $m_\pm = n$ iff the indicated homogeneous equation has the maximum number n of linearly independent square-integrable solutions for any W, in particular, with any real $W = E$. It follows from this general statement that to have the deficiency indices $m_\pm = 1$, in our particular case where $n = 2$, it suffices to point out the conditions on $V(x)$ under which the homogeneous equation $(\check{H} - W)u = 0$ on the semiaxis $\mathbb{R}_+$ has at least one non-square-integrable solution. Some such conditions have been known since Weyl; see [162].

Let now the s.a. differential operation $\check{H}$ be given on the whole real axis $\mathbb{R}$, and suppose that the potential $V(x)$ satisfies condition (7.3) or (7.4) on ∞ and condition (7.13) or (7.14) on $-\infty$. Because in such a case the boundary forms at the infinite endpoints $\pm\infty$ are zero, and the quadratic form $\Delta_H(\psi_*)$ is zero as well, there exists a unique s.a. extension $\hat{H}_\mathfrak{e}$ of the initial symmetric operator $\hat{H}$, which is $\hat{H}_\mathfrak{e} = \hat{H}^+$, $D_{H_\mathfrak{e}} = D^*_{\check{H}}(\mathbb{R})$. The case of a free particle certainly falls under these conditions, so that the Hamiltonian $\widehat{\mathcal{H}}_\mathfrak{e}$ associated with $\check{\mathcal{H}}$ and defined on the natural domain is truly s.a., as was demonstrated in Chap. 6. The majority of the potentials encountered in physics satisfy these conditions, so that the above assertion implicitly adopted in physics textbooks is actually justified. In particular, this concerns one-dimensional Hamiltonians with bounded potentials such as a potential barrier, a potential well of finite depth, or with the exactly solvable potentials such as $V_0\mathrm{ch}^{-2}(ax)$ and also concerns Hamiltonians with potentials growing at infinity, for example, the Hamiltonian of a harmonic oscillator, in which case $\check{H} = \check{\mathcal{H}} + x^2$, and even a Hamiltonian with linear potential $V(x) = kx$ that tends to $-\infty$ at one of the endpoints, but only linearly and not faster then quadratically; see Chap. 8.

7.1.3 Third Remark

The majority of potentials encountered in physics, in particular, potentials decreasing or growing at infinity, satisfy condition (7.4). This condition is optimum in the sense that if $V(x) \backsim -Kx^{2(1+\varepsilon)}$ as $x \to \infty$, where $\varepsilon > 0$ can be arbitrarily small, then both linearly independent solutions $u_{1,2}$ of the Schrödinger equation (7.2) with any W are square-integrable at infinity:

$$u_{\pm}(x) \backsim x^{-(1+\varepsilon)/2} \exp\left[\pm i \frac{K^{1/2}}{2+\varepsilon} x^{2+\varepsilon}\right],\ x \to \infty,$$

and the s.a. boundary conditions must include the boundary conditions at infinity. This fact is crucial in the sense that ignoring it results in a "paradox." If we directly, without thinking about it, proceed to solving (7.2), which not infrequently happens in physics texts, we find ourselves in a situation in which for any energy E this equation has solutions square-integrable on the semiaxis and corresponding to the bound states. From a naïve standpoint, this means that all the eigenstates in such a potential are bound, and what is more, the spectrum of such states, which must be discrete, turns out to be continuous, which is an absurdity! This situation[4] is similar to the case of "the fall to the center" for a particle of negative energy in the strongly attractive potential $V(x) \leq \alpha x^{-2}$, $\alpha < -1/4$ as $x \to 0$, see [5, 21, 118, 123, 151]. The resolution of this paradox lies in the necessity of the s.a. boundary conditions at infinity in addition to the customary boundary conditions at the origin; without these boundary conditions, we are in fact dealing with the "Hamiltonian" $\hat{H}^* = \hat{H}^+$, which is not s.a. Taking only the s.a. boundary conditions at infinity into account, we obtain an s.a. Hamiltonian all of whose eigenstates are bound states, and the spectrum is discrete.

To all this we add a remark concerning the s.a. differential operation (7.1) defined on the interval $[0, l]$. The remark is that s.a. operators $\hat{H}_U$ associated with this differential operation are specified by the same s.a. boundary conditions (6.28) as the operators $\widehat{\mathcal{H}}_U$ if the potential $V(x)$ is integrable on the interval, because under this condition, the s.a. differential operation $\check{H}$ remains regular and the asymmetry form ω_{H^+} does not change. This is all the more clear in the case that the potential is bounded, $|V(x)| < M$, because the addition of a bounded s.a. operator defined everywhere to any s.a. operator yields the s.a. operator with the same domain.

In the following chapters, we consider examples of singular endpoints for which the boundary form is nontrivial.

[4] It can be called "the fall to infinity" because a classical particle goes out to infinity in a finite time.

7.2 The Calogero Problem

7.2.1 Introduction

Here we consider the potential field

$$V(x) = \alpha x^{-2} \tag{7.15}$$

in (7.1) and (7.2), singular at the origin. The case of $\alpha > 0$ corresponds to a repulsion potential (repulsion from the origin); the case of $\alpha < 0$ corresponds to an attraction potential (attraction to the origin). Our considerations are based on our work [76].

Starting from the basic papers by Calogero on the exactly solvable one-dimensional QM models [34–36], the potential (7.15) is conventionally called the *Calogero potential* and the problem of QM description of the system is known as the *Calogero problem*. In fact, Calogero considered a more general case with quadratic and inversely quadratic terms in $V(x)$. We call such a potential the *generalized Calogero potential*. Self-adjoint Schrödinger operators with such a potential are considered in Sect. 8.4. Physicists identify the corresponding differential operation (7.1) with a radial "Hamiltonian"; see Sect. 4.3. Such a potential causes the phenomenon that is known as "the fall to the center", see [5, 21, 118, 123, 151]. Historically, it is the potential with which the first case is associated, whereby the standard physical approach did not allow the construction of the scattering states because of an unusual uncertainty in the choice of the behavior of the wave functions at the origin, and even the question arose whether QM is applicable to systems with strongly attractive potentials [115]. Since then, the QM problem with the potential αx^{-2} has been discussed repeatedly and in various aspects; see, for example, [12, 38, 111]. And the discussion continues.

We restrict ourselves here to the case of a motion on a semiaxis[5] $\mathbb{R}_+$. The case can be considered the problem of a radial motion (with $x \to r$) of a particle in higher dimensions in a potential field $\sim r^{-2}$; see for example Chap. 9. The peculiarity of higher-dimensional classical mechanics in the case of attraction is that under some initial conditions the particle "falls to the center" in a finite time interval, see [103], so that the final state at the endpoint of this interval is a position $\mathbf{r} = 0$ and a momentum $|\mathbf{p}| = \infty$ of uncertain direction, and the problem arises how to define the motion of the particle after this time interval. In some sense, QM "inherits" these difficulties, although it gives them a QM form.

We first discuss QM paradoxes related to singular potentials on the example of the problem under consideration.

[5]The case of the whole axis $\mathbb{R}$ can be considered by the same methods. We mention only that the corresponding QM contains more ambiguity.

7.2.2 A "Naïve" Treatment of the Problem and Related Paradoxes

Here we start with the *Calogero differential operation* defined as

$$\check{H} = -d_x^2 + \alpha x^{-2}. \tag{7.16}$$

In the x-representation, the Hilbert space of QM states for the Calogero problem is $\mathfrak{H} = L^2(\mathbb{R}_+)$, and in the naïve consideration, the Calogero Hamiltonian $\hat{H}$ is identified with the apparent s.a. operator (7.16) in $L^2(\mathbb{R}_+)$ for any α, because it is the sum of what are certainly two s.a. operators $-d_x^2$ and $\hat{V} = \alpha x^{-2}$, although $\hat{V}$ is unbounded if $\alpha \neq 0$; we say in advance that the latter is precisely the reason for paradoxes.

In QM with such an understood Calogero Hamiltonian $\hat{H}$, the time evolution is unitary and is defined for all moments of time, although an analogue of "the fall to the center" is well known from textbooks for $\alpha < -1/4$: in this case, the spectrum of $\hat{H}$ is unbounded from below (although the spectrum itself as well as eigenfunctions are not presented; see [104]). This is argued by considering the Calogero potential as a limit of bounded regularized potentials:

$$V_{r_0}(x) = \begin{cases} \alpha x^{-2}, & x \geq r_0, \\ \alpha r_0^{-2}, & x < r_0, \end{cases} \tag{7.17}$$

with $r_0 \to 0$. To be sure, the limit ($r_0 \to 0$) spectrum is not presented; moreover, the attentive reader can see that there is no limit spectrum, so that the problem of the spectrum as well as limit eigenfunctions of the Calogero Hamiltonian in the case $\alpha < -1/4$ remains completely open.

Let us look at the problem in more detail. It is natural to expect that for $\alpha \geq 0$, the spectrum of $\hat{H}$ is nonnegative, and no bound states exist. Let $\alpha < 0$. Because any symmetric one-dimensional well "traps" a particle, we expect that there must be a negative energy level $E_0 < 0$ in addition to the nonnegative spectrum.

We now turn to some symmetry arguments. It seems evident that the Calogero Hamiltonian has scale symmetry: under the scale transformations $x \to x' = lx$, $l > 0$, the operators $\widehat{\mathcal{H}} = -d_x^2$ and $\hat{V} = \alpha x^{-2}$ transform uniformly and are of the same spatial dimension, $\mathrm{d}_{H_0} = \mathrm{d}_V = -2$; therefore, the operator $\hat{H}$ also transforms uniformly under scale transformations, and $\mathrm{d}_H = -2$. This observation is formalized as follows.

We consider the group of scale transformations $x \to x' = lx$, $x \in \mathbb{R}_+$, $\forall l > 0$, and its unitary representation in $L^2(\mathbb{R}_+)$, the space of quantum states by unitary operators $\hat{U}(l)$,

$$\hat{U}(l)\,\psi(x) = l^{-1/2}\psi\left(l^{-1}x\right) \tag{7.18}$$

(the spatial dimension d_ψ of wave functions $\psi(x)$ is $\mathrm{d}_\psi = -1/2$ because $|\psi(x)|^2$ is the spatial probability density). The unitarity of $\hat{U}(l)$ is easily verified,

$$\left\|\hat{U}(l)\psi\right\| = \int_{-\infty}^{+\infty} \mathrm{d}x l^{-1} \left|\psi\left(l^{-1}x\right)\right|^2 = \int_{-\infty}^{+\infty} \mathrm{d}x\, |\psi(x)|^2 = \|\psi\|^2,$$

as well as the group law $\hat{U}(l_2)\hat{U}(l_1) = \hat{U}(l_2 l_1)$. It is also easily verified that

$$\hat{H}\hat{U}(l) = l^{-2}\hat{U}(l)\hat{H} \Longleftrightarrow \hat{U}^{-1}(l)\hat{H}\hat{U}(l) = l^{-2}\hat{H}, \tag{7.19}$$

or $\mathrm{d}_H = -2$.

For completeness, we present the infinitesimal version of the scale symmetry. The unitary scale transformations $\hat{U}(l)$ can be presented as

$$\hat{U}(l) = \exp\left(i \ln l \hat{D}\right), \quad \hat{D} = ixd_x + i/2,$$

where $\hat{D}$ is the s.a. generator of the scale transformations. The scale symmetry algebra for the Hamiltonian $\hat{H}$ is $[\hat{D}, \hat{H}] = -2i\hat{H}$.

Let now $\psi_E(x)$ be an eigenfunction of $\hat{H}$ with an eigenvalue E, then the scale-symmetry operator relation (7.19) applied to this function yields

$$\hat{H}\left[\hat{U}(l)\psi_E(x)\right] = l^{-2}\hat{U}(l)\hat{H}\psi_E(x) = \left(l^{-2}E\right)\hat{U}(l)\psi_E(x),$$

which implies that $\hat{U}(l)\psi_E(x) = \psi_{l^{-2}E}(x)$, $\forall l > 0$, is an eigenfunction of $\hat{H}$ with the eigenvalue $l^{-2}E$. But this means that the group of scale transformations acts transitively on both positive and negative parts of the energy spectrum such that these parts must either be empty or fill the respective positive and negative semiaxis of the real axis.

This is completely consistent with what we expect for the spectrum of $\hat{H}$ in the case of repulsion, $\alpha > 0$ where $E \geq 0$.

But in the case of attraction, $\alpha < 0$, we meet paradoxes. Indeed, for $\alpha < 0$, we expect at least one negative level $E_0 < 0$. But if there is at least one such level, then, according to the scale symmetry, there must be a continuous set of normalized eigenstates with the energies $l^{-2}E_0$, $\forall l > 0$, and the negative part of the spectrum is the whole negative semiaxis, and "the fall to the center" occurs for all $\alpha < 0$.

This picture is quite unusual and contradictory, because there can be no continuous set of normalizable eigenstates for any s.a. operator in $L^2(\mathbb{R}_+)$: it would contradict the fact that $L^2(\mathbb{R}_+)$ is a separable Hilbert space. Another surprising fact is that the spectrum of the Calogero Hamiltonian is not bounded from below for any $\alpha < 0$, not only for $\alpha < -1/4$.

The situation becomes even more entangled if we try to find bound states of $\hat{H}$ corresponding to negative energy levels, $E < 0$. The corresponding differential equation for these eigenstates $\psi_E(x) \equiv \psi_k(x)$ is

$$\check{H}\psi_k(x) = -k^2\psi_k(x), \, k^2 = -E > 0. \tag{7.20}$$

There are two “dangerous” points for the square-integrability of $\psi_k(x)$: infinity, $x = \infty$, and the origin, $x = 0$, which is a point of singularity of the potential and a boundary simultaneously.

The behavior of a solution $\psi_k(x)$, if it exists, at infinity is evident: $\psi_k(x) \sim c \exp(-kx)$ as $x \to \infty$.

The behavior of a solution $\psi_k(x)$, if it exists, at infinity where the potential vanishes is evident: $\psi_k(x) \simeq c \exp(-kx)$, $x \to \infty$. This behavior, which manifests the square-integrability of $\psi_k(x)$ at infinity, must be compatible with the local square-integrability of $\psi_k(x)$ at the origin. The existence of $\psi_k(x)$ for a given k is thus defined by its asymptotic behavior at the origin, which, because of the singularity, coincides with the asymptotic behavior of the general solution of the homogeneous equation $\check{H}y(x) = 0$ at the origin. The general solution of this equation is

$$y(x) = \begin{cases} x^{1/2}(c_1 x^{\varkappa} + c_2 x^{-\varkappa}), \, \alpha \neq -1/4, \\ x^{1/2}(c_1 + c_2 \ln x), \, \alpha = -1/4, \end{cases}$$

where

$$\varkappa = \sqrt{1/4 + \alpha} = \begin{cases} \sqrt[+]{1/4+\alpha}, \, \alpha \geq -1/4, \\ i\sigma, \, \sigma = \sqrt{|1/4+\alpha|}, \, \alpha < -1/4. \end{cases}$$

We can see that if $-1/4 \leq \alpha < 0$, we have $\varkappa < 1/2$, and $y(x) \to 0$ as $x \to 0$, so that $\psi_k(x)$ is certainly square-integrable at the origin irrespective of k. The same holds true if $\alpha < -1/4$, in which case $\varkappa = i\sigma$ and $y(x) \to 0$ infinitely oscillating as $x \to 0$. This implies that $\psi_k(x)$ exists for any $k > 0$, which confirms the previous arguments that the negative “discrete” spectrum is in fact continuous and occupies all the negative real semiaxis.

Furthermore, both functions $x^{1/2 \pm \varkappa}$ are also square-integrable if $1/2 \leq \varkappa < 1$, i.e., if $0 \leq \alpha < 3/4$, so that there is a continuous set of negative energy levels unbounded from below for $\alpha = 0$ (the case of a free particle) and even for repulsive potentials, $V(x) > 0$. “The fall to the center” for repulsive potentials is quite paradoxical.

We can present an explicit form of $\psi_k(x)$. By the substitution $\psi_k(x) = x^{1/2}u_k(kx)$, we reduce (7.20) to the following equation for the function $u(z) = u_k(kx)$, $z = kx$:

$$u'' + z^{-1}u - (1 + \varkappa^2 z^{-2})u = 0,$$

whose solutions are the Bessel functions of imaginary argument. It follows that for $\alpha < 3/4$ and for any $k > 0$ the square-integrable solution of the eigenvalue problem (7.20) for bound states is given by $\psi_k(x) = x^{1/2}K_{\varkappa}(kx)$, where $K_{\varkappa}(x)$ is the so-called McDonald function.

Our final remark is that $\psi_k(x)$ remains square-integrable for complex $k = k_1 + ik_2,\ k_1 > 0$, so that the seemingly s.a. $\hat{H}$ has complex eigenvalues.

These inconsistencies, or paradoxes, reveal that something is wrong with QM in the case of singular potentials, as well as in the case of boundaries, or at least something is wrong with our previous considerations following the conventional methods. It appears that we have been too "naïve" in our considerations; strictly speaking, we have been incorrect, and our arguments have been wrong. The main reason is that almost all operators involved are unbounded, while for unbounded operators, in contrast to bounded operators defined everywhere, the algebraic rules, the notions of self-adjointness, commutativity, and symmetry are nontrivial.

In particular, we actually implicitly adopted that the operator $\hat{H}$ acts (is defined) on the so-called natural domain, which is the set of square-integrable functions ψ satisfying only the conditions that the differential operation $\check{H}$ is applicable to ψ and $\check{H}\psi$ is also square-integrable.

As we shall see below, this operator with $\alpha < 3/4$ is not s.a.

7.2.3 Self-adjoint Calogero Hamiltonians

We now proceed with a more rigorous QM treatment of the Calogero problem on the semiaxis $\mathbb{R}_+$. The first problem to be solved is constructing and suitably specifying all Calogero Hamiltonians as s.a. operators in the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}_+)$; the second problem is a complete spectral analysis of each of the obtained Hamiltonians, and finally, resolving the paradoxes discussed in the previous section, in particular, the paradox concerning the apparent scale symmetry.

We are going to be brief when presenting the main steps of the solution. The details can be easily elaborated.

We start with the differential operation (7.16) to construct the initial symmetric operator $\hat{H}$, its adjoint $\hat{H}^+$, and s.a. extensions of $\hat{H}$. All these operators differ by their domains, while their action on the corresponding domains is given by the same differential operation (7.16). When defining these operators in what follows, we therefore cite only their domains.

The domain D_H of the initial symmetric operator $\hat{H}$ is the linear space $\mathcal{D}(\mathbb{R}_+)$. The domain D_{H^+} of the operator $\hat{H}^+$ is the natural domain for $\check{H}$, i.e., $D_{H^+} = D^*_{\check{H}}(\mathbb{R}_+)$; see (4.29).

In constructing s.a. extensions of the operator $\hat{H}$, we will apply the method that uses the asymmetry form $\Delta_{H^+}(\psi_*)$, where $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$; see Chaps. 3 and 4. In the case under consideration, the asymmetry form is given by

$$\Delta_{H^+}(\psi_*) = \lim_{\substack{\varepsilon\to 0\\ L\to\infty}} \left(\overline{\psi_*'}\psi_* - \overline{\psi_*}\psi_*'\right)\Big|_\varepsilon^L .$$

The further specification of Δ_{H+} requires the knowledge of the behavior of the wave functions ψ_* and ψ_*' near the origin and at infinity.

Regarding infinity, we assert that

$$\psi_* \in D_{\check{H}}^* (\mathbb{R}_+) \Longrightarrow \psi_* (x), \psi_*' (x) \overset{x\to\infty}{\longrightarrow} 0. \tag{7.21}$$

This is proved similarly to the free particle case, see Lemmas 2.13 and 2.14, in view of the fact that if $\psi_*(x)$ and $\check{H}\psi_*(x)$ are square-integrable at infinity, then $\psi_*'' (x) = \alpha x^{-2}\psi_*(x) - \check{H}\psi_*(x)$ is also square-integrable at infinity.

As for the behavior of ψ_* and ψ_*' near the origin, it is established as follows: Let us consider the relation

$$\check{H}\psi_* = \chi \in L^2 (\mathbb{R}_+) \tag{7.22}$$

as a differential equation with respect to the function ψ_* via a given χ. The general solution of this equation for $\alpha \neq -1/4$ ($\varkappa \neq 0$) can be represented in the form

$$\begin{aligned}
\psi_*(x) &= c_1 (k_0 x)^{1/2+\varkappa} + c_2 (k_0 x)^{1/2-\varkappa} \\
&\quad + \frac{x^{1/2}}{2\varkappa}\left[x^{-\varkappa}\int_0^x \mathrm{d}y\, y^{1/2+\varkappa}\chi - x^{\varkappa}\int_a^x \mathrm{d}y\, y^{1/2-\varkappa}\chi\right], \\
\psi_*'(x) &= \left[c_1 (k_0 x)^{1/2+\varkappa} + c_2 (k_0 x)^{1/2-\varkappa}\right]' + \frac{x^{-1/2}}{2\varkappa} \\
&\quad \times \left[(1/2-\varkappa)\, x^{-\varkappa}\int_0^x \mathrm{d}y\, y^{1/2+\varkappa}\chi - (1/2+\varkappa)\, x^{\varkappa}\int_a^x \mathrm{d}y\, y^{1/2-\varkappa}\chi\right],
\end{aligned} \tag{7.23}$$

where k_0 is an arbitrary but fixed parameter of dimensionality of inverse length introduced for dimensional reasons; $a > 0$ for $\alpha \geq 3/4$, and $a = 0$ for $\alpha < 3/4$. The case $\alpha = -1/4 \Longleftrightarrow \varkappa = 0$ is considered below.

We now estimate the behavior of the integral terms in (7.23) near the origin using the Cauchy–Schwarz inequality. For example, if $\alpha > -1/4 \Longleftrightarrow \varkappa > 0$, we have

$$\left|x^{1/2-\varkappa}\int_a^x \mathrm{d}y\, y^{1/2+\varkappa}\chi\right| \leq x^{1/2-\varkappa}\left[\int_0^x \mathrm{d}y\, y^{1+2\varkappa}\right]^{1/2}\left[\int_0^x \mathrm{d}y\, |\chi|^2\right]^{1/2}. \tag{7.24}$$

The integrals on the right-hand side of (7.24) vanish as $x \to 0$. More precisely

$$\left[\int_0^x \mathrm{d}y\, y^{1+2\varkappa}\right]^{1/2} = O\left(x^{1+\varkappa}\right), \left[\int_0^x \mathrm{d}y\, |\chi|^2\right]^{1/2} \overset{x\to 0}{\longrightarrow} 0.$$

The second estimate follows from the fact that $\chi \in L^2(\mathbb{R}_+)$. Then

$$\left|x^{1/2-\varkappa}\int_0^x \mathrm{d}y\, y^{1/2+\varkappa}\chi\right| \leq O(x^{3/2}).$$

We thus obtain the behavior of ψ_* near the origin (we recall that $\alpha \neq -1/4$),

$$\psi_*(x) = \psi_*^{\mathrm{as}}(x) + \begin{cases} O(x^{3/2}), \ \alpha \neq 3/4, \\ O(x^{3/2}\sqrt{\ln x}), \ \alpha = 3/4, \end{cases}$$

$$\psi_*'(x) = \psi_*^{\mathrm{as}\prime}(x) + \begin{cases} O(x^{1/2}), \ \alpha \neq 3/4, \\ O(x^{1/2}\sqrt{\ln x}), \ \alpha = 3/4, \end{cases} \tag{7.25}$$

where

$$\psi_*^{\mathrm{as}}(x) = c_1 (k_0 x)^{1/2+\varkappa} + c_2 (k_0 x)^{1/2-\varkappa} .$$

We stress that estimates for $\psi_*(x)$ and $\psi_*'(x)$ are performed independently. We now recall that $\psi_* \in L^2(\mathbb{R}_+)$, which requires that $c_2 = 0$ for $\alpha \geq 3/4$ ($\varkappa \geq 1\}$, because the term $c_2 (k_0 x)^{1/2-\varkappa}$ is not square-integrable at zero unless $c_2 = 0$. Furthermore, for $\alpha \geq 3/4$, the term $c_1 (k_0 x)^{1/2+\varkappa}$ in $\psi_*^{\mathrm{as}}(x)$ can be included in the remainder term $O(x^{3/2})$ in (7.25). We thus can assume $c_1 = c_2 = 0$ for $\alpha \geq 3/4$.

The general solution of (7.22) for $\alpha = -1/4$ is

$$\begin{aligned}
\psi_*(x) &= c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x) + x^{1/2}\int_0^x dy\,\Theta(y)'\ln(k_0 y) \\
&\quad - x^{1/2}\ln(k_0 x)\Theta(x) = -x^{1/2}\int_0^x dy\,y^{-1}\Theta(y) + c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x), \\
\psi_*'(x) &= [c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x)]' - [x^{1/2}\ln(k_0 x)]'\Theta(x) \\
&\quad + 2^{-1}x^{-1/2}\int_0^x dy\,\Theta(y)'\ln(k_0 y) = [c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x)]' \\
&\quad - 2^{-1}x^{-1/2}\int_0^x dy\,y^{-1}\Theta(y) - x^{-1/2}\Theta(x), \\
\Theta(x) &= \int_0^x dy\,y^{1/2}\chi(y), \ |\Theta(x)| = O(x), \ x \to 0,
\end{aligned}$$

which implies the following behavior as $x \to 0$:

$$\begin{aligned}
&\psi_*(x) = \psi_*^{\mathrm{as}}(x) + O(x^{3/2}), \ \psi_*'(x) = \psi_*^{\mathrm{as}\prime}(x) + O(x^{1/2}), \\
&\psi_*^{\mathrm{as}}(x) = c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x) .
\end{aligned} \tag{7.26}$$

With these estimates in hand, we can specify the asymmetry form Δ_{H+} in terms of the asymptotic behavior of ψ_* at the origin; infinity appears to be irrelevant as in the case of a free particle. It is natural because the potential vanishes at infinity.

The result essentially depends on the coupling constant α, and we distinguish four cases.

7.2.3.1 The First Region $\alpha \geq 3/4$

In this region $\varkappa \geq 1$. Taking into account (7.25) and (7.23), and the fact that $c_1 = c_2 = 0$ in the region under consideration, we get $\Delta_{H+} = 0$. It follows that the deficiency indices of $\hat{H}$ in this case are zero, and therefore $\hat{H}$ is essentially s.a., and its unique s.a. extension, we denote it by $\hat{H}_1$, is $\hat{H}_1 = \hat{H}^+$. Thus, in the case under consideration, there exists only one s.a. Calogero Hamiltonian $\hat{H}_1$ defined on the domain $D_{H_1} = D^*_{\check{H}}(\mathbb{R}_+)$. As follows from the above estimates at $\alpha \geq 3/4$, the functions $\psi_*(x) \in D^*_{\check{H}}(\mathbb{R}_+)$ satisfy a.b. conditions as $x \to 0$,

$$\psi_*(x) = O(x^{3/2}),\ \psi_*'(x) = O(x^{1/2}),\ \alpha > 3/4,$$
$$\psi_*(x) = O(x^{3/2}\sqrt{\ln x}),\ \psi_*'(x) = O(x^{1/2}\sqrt{\ln x}),\ \alpha = 3/4.$$

7.2.3.2 The Second Region $-1/4 < \alpha < 3/4$

In this region $0 < \varkappa < 1$, and the asymmetry form Δ_{H+} is calculated with the help of (7.25) and (7.21),

$$\Delta_{H+}(\psi_*) = 2k_0\varkappa\,(\overline{c_2}c_1 - \overline{c_1}c_2) = ik_0\varkappa\left(|c_+|^2 - |c_-|^2\right),\ c_\pm = c_1 \pm ic_2.$$

Restrictions on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$ follow from the condition $\Delta_{H+}(\psi_*) = 0$, which implies $c_- = e^{i\vartheta}c_+$, $\vartheta \in \mathbb{S}(0, 2\pi)$, or equivalently

$$c_2 \cos\nu = c_1 \sin\nu,\ \nu = \vartheta/2 - \pi/2 \in \mathbb{S}(-\pi/2, \pi/2). \tag{7.27}$$

According to (7.25) and (7.21), relation (7.27) specifies a.b. conditions as $x \to 0$,

$$\psi_\nu(x) = C\psi_\nu^{\mathrm{as}}(x) + O(x^{3/2}),\ \psi_\nu'(x) = C\psi_\nu^{\mathrm{as}\prime}(x) + O(x^{1/2}),$$
$$\psi_\nu^{\mathrm{as}}(x) = (k_0x)^{1/2+\varkappa}\sin\nu + (k_0x)^{1/2-\varkappa}\cos\nu. \tag{7.28}$$

It follows that in this case the deficiency indices of $\hat{H}$ are $m_\pm = 1$. Therefore, in the case under consideration, there exists a one-parameter $U(1)$ family of s.a. extensions $\hat{H}_{2,\nu}$ of the initial symmetric operator $\hat{H}$, specified by their domains $D_{H_{2,\nu}}$,

$$D_{H_{2,\nu}} = \left\{\psi_\nu : \psi_\nu \in D^*_{\check{H}}(\mathbb{R}_+)\,;\ \psi_\nu \text{ obey } (7.28)\right\}. \tag{7.29}$$

7.2.3.3 The Third Region $\alpha = -1/4$

In this region $\varkappa = 0$. Taking into account (7.26) and (7.21), we obtain

$$\varDelta_{H^+}(\psi_*) = -k_0\left(\overline{c_1}c_2 - \overline{c_2}c_1\right) = \frac{i}{2}k_0\left(|c_+|^2 - |c_-|^2\right),\ c_\pm = c_1 \pm ic_2\,.$$

Restrictions on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$ follow from the condition $\varDelta_{H^+}(\psi_*) = 0$, which implies $c_- = \mathrm{e}^{i\vartheta}c_+$, $\vartheta \in \mathbb{S}(0, 2\pi)$, or equivalently

$$c_2\cos\nu = c_1\sin\nu,\ \nu = \vartheta/2 - \pi/2 \in \mathbb{S}(-\pi/2, \pi/2)\,. \tag{7.30}$$

According to (7.26), relation (7.30) defines a.b. conditions for functions $\psi_\nu(x)$ from $D^*_{\check{H}}(\mathbb{R}_+)$ as $x \to 0$,

$$\begin{aligned}&\psi_\nu(x) = C\psi_\nu^{\mathrm{as}}(x) + O(x^{3/2}),\ \psi_\nu'(x) = C\psi_\nu^{\mathrm{as}\prime}(x) + O(x^{1/2}),\\ &\psi_\lambda^{\mathrm{as}}(x) = x^{1/2}\sin\nu + x^{1/2}\ln(k_0x)\cos\nu.\end{aligned} \tag{7.31}$$

It follows that in this case the deficiency indices of $\hat{H}$ are $m_\pm = 1$. Therefore, in the case under consideration, there exists a one-parameter $U(1)$ family of s.a. extensions $\hat{H}_{3,\nu}$ of the initial symmetric operator $\hat{H}$, specified by their domains $D_{H_{3,\nu}}$,

$$D_{H_{3,\nu}} = \left\{\psi_\nu : \psi_\nu \in D^*_{\check{H}}(\mathbb{R}_+)\,;\ \psi_\nu \text{ obey } (7.31)\right\}. \tag{7.32}$$

7.2.3.4 The Fourth Region $\alpha < -1/4$

In this region $\varkappa = i\sigma, \sigma > 0$. The asymptotic behavior of the general solution at the origin is given by (7.23). Taking it into account, we obtain

$$\varDelta_{H^+}(\psi_*) = i2k_0\sigma\left(|c_1|^2 - |c_2|^2\right).$$

Restrictions on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$ follow from the condition $\varDelta_{H^+}(\psi_*) = 0$, which implies $\mathrm{e}^{i\theta}c_2 = \mathrm{e}^{-i\theta}c_1$, $\theta \in \mathbb{S}(0, \pi)$. According to (7.23), this defines s.a. boundary conditions for functions $\psi_\theta(x)$ from $D^*_{\check{H}}(\mathbb{R}_+)$ as $x \to 0$,

$$\begin{aligned}&\psi_\theta(x) = C\psi_\theta^{\mathrm{as}}(x) + O(x^{3/2}),\ \ \psi_\theta'(x) = C\psi_\theta^{\mathrm{as}\prime}(x) + O(x^{1/2}),\\ &\psi_\theta^{\mathrm{as}}(x) = x^{1/2}\left[\mathrm{e}^{i\theta}(k_0x)^{i\sigma} + \mathrm{e}^{-i\theta}(k_0x)^{-i\sigma}\right].\end{aligned} \tag{7.33}$$

It follows that in this case the deficiency indices of $\hat{H}$ are $m_\pm = 1$. Therefore, in the case under consideration, there exists a one-parameter $U(1)$ family of s.a.

extensions $\hat{H}_{4,\theta}$, $\theta \in \mathbb{S}(0,\pi)$ of the initial symmetric operator $\hat{H}$, specified by their domains $D_{H_{4,\theta}}$,

$$D_{H_{4,\theta}} = \left\{ \psi_\theta : \psi_\theta \in D^*_{\check{H}}(\mathbb{R}_+) ;\ \psi_\theta \text{ obey } (7.33) \right\}. \tag{7.34}$$

7.2.4 Spectral Problem and Inversion Formulas

We follow Chap. 5 in solving the spectral problem and finding inversion formulas.

Let us we construct a Green's function $G(x, y; W)$ of s.a. Calogero Hamiltonians $\hat{H}_a$, $a = 1, 2, 3, 4$. As follows from Sect. 5.3.4, we have first to find the general solutions of the inhomogeneous equation

$$(\check{H} - W)\psi = \eta \in L^2(\mathbb{R}_+),\ W = |W|e^{i\varphi},\ 0 \le \varphi \le \pi,\ \operatorname{Im} W > 0. \tag{7.35}$$

To this end, we first consider the corresponding homogeneous equation

$$(\check{H} - W)\psi = 0, \tag{7.36}$$

and a set $u_i(x; W)$, $i = 1, 2$, and $v_1(x; W)$ of its solutions,

$$u_1(x; W) = \Gamma(1+\varkappa)(\beta/2k_0)^{-\varkappa}(k_0x)^{1/2} J_\varkappa(\beta x),$$

$$u_2(x; W) = \Gamma(1-\varkappa)(\beta/2k_0)^{\varkappa}(k_0x)^{1/2} J_{-\varkappa}(\beta x)$$

$$\begin{aligned} v_1(x; W) &= (\beta/2k_0)^{\varkappa}(k_0x)^{1/2} H^{(1)}_\varkappa(\beta x) \\ &= -\frac{i}{\pi}\left(e^{-i\pi/2}\beta/2k_0\right)^{2\varkappa}\Gamma(-\varkappa)u_1(x; W) - \frac{i\Gamma(\varkappa)}{\pi}u_2(x; W), \end{aligned}$$

where $\beta = \sqrt{W} = e^{i\varphi/2}\sqrt{|W|}$, $\operatorname{Im}\beta > 0$, and $J_\varkappa(x)$ and $H^{(1)}_\varkappa(x)$ are the Bessel and Hankel functions respectively; see [1, 20, 81]. Note that the functions $u_1(x; W)$ and $u_2(x; W)$ are entire in W, are real entire in W for $\alpha \ge -1/4$ ($\varkappa \ge 0$), and satisfy the relation $u_2(x; E) = \overline{u_1(x; E)}$ for $\alpha < -1/4$ ($\varkappa = i\sigma$). The function $v_1(x; W)$ is analytic in the upper half-plane.

As $x \to \infty$, $\operatorname{Im} W > 0$, we have

$$\begin{aligned} u_1(x; W) &= \frac{\Gamma(1+\varkappa)}{2\sqrt{\pi}}(\beta/2k_0)^{-1/2-\varkappa} e^{-i(\beta x - \varkappa\pi/2 - \pi/4)}\tilde{O}(x^{-1}) \to \infty, \\ v_1(x; W) &= \frac{2k_0}{\sqrt{\pi}\beta}(\beta/2k_0)^{1/2+\varkappa} e^{i(\beta x - \varkappa\pi/2 - \pi/4)}\tilde{O}(x^{-1}) \to 0, \end{aligned} \tag{7.37}$$

and thus the solution $v_1(x;W)$ is square-integrable at infinity for $\operatorname{Im} W > 0$. As $x \to 0$, we have

$$u_1(x;W) = (k_0 x)^{1/2+\varkappa}\tilde{O}(x^2),\ u_2(x;W) = (k_0 x)^{1/2-\varkappa}\tilde{O}(x^2),\ v_1(x;W)$$
$$= \begin{cases} -\frac{i\Gamma(\varkappa)}{\pi}(k_0 x)^{1/2-\varkappa}\tilde{O}(x^2),\ \alpha \geq 3/4, \\ -\frac{i\Gamma(\varkappa)}{\pi}(k_0 x)^{1/2-\varkappa}\tilde{O}(x^2), \\ -i\mathrm{e}^{-i\pi\varkappa}\frac{\Gamma(-\varkappa)}{\pi}(\beta/2k_0)^{2\varkappa}(k_0 x)^{1/2+\varkappa},\ \ \alpha < 3/4,\ \alpha \neq -1/4, \\ \frac{2i(k_0 x)^{1/2}}{\pi}\left[\pi/2i + \mathbf{C} + \ln(\beta/2k_0) + \ln(k_0 x)\right]\tilde{O}(x^2),\ \alpha = -1/4, \end{cases} \tag{7.38}$$

where $\mathbf{C}$ is Euler's constant.

The Wronskians of the solutions u_1, u_2, and v_1 are

$$\operatorname{Wr}(u_1, u_2) = -2k_0\varkappa,\ \operatorname{Wr}(u_1, v_1) = 2i\pi^{-1}k_0\Gamma(1+\varkappa).$$

Then the general solution of (7.35) has the form

$$\psi(x) = a_1 u_1(x;W) + a_2 v_1(x;W) + \frac{i\pi}{2k_0\Gamma(1+\varkappa)}$$
$$\times\left[\int_x^\infty G_1^{(+)}(x,y;W)\eta(y)\mathrm{d}y + \int_0^x G_1^{(-)}(x,y;W)\eta(y)\mathrm{d}y\right], \tag{7.39}$$

where

$$G_1^{(+)}(x,y;W) = u_1(x;W)v_1(y;W),$$
$$G_1^{(-)}(x,y;W) = v_1(x;W)u_1(y;W).$$

To find solutions $\psi \in D_{H_a}$, one needs to determine coefficients a_1 and a_2, using first the condition $\psi \in L^2(\mathbb{R}_+)$ and then s.a. boundary conditions as $x \to 0$ that specify the domains D_{H_a}.

With the help of the Cauchy–Schwarz inequality, we can easily estimate integral summands on the right-hand side of (7.39). These terms, as well as the term $a_2 v_1$, are restricted as $x \to \infty$. Therefore the condition $\psi \in L^2(\mathbb{R}_+)$ implies $a_1 = 0$.

7.2.4.1 The First Region $\alpha \geq 3/4$

In this region, $\varkappa \geq 1$ and there exists only one s.a. Calogero Hamiltonian $\hat{H}_1$ defined on the domain $D_{H_1} = D^*_{\check{H}}(\mathbb{R}_+)$.

For $\alpha \geq 3/4$, with the help of the Cauchy–Schwarz inequality, we find that the integral summands in (7.39) are restricted as $x \to 0$ (in fact, they vanish in such a limit), so that the condition $\psi \in L^2(\mathbb{R}_+)$ implies $a_2 = 0$ and the Green's function of the Hamiltonian $\hat{H}_1$ reads

$$G(x, y; W) = \frac{i\pi}{2k_0\Gamma(1+\varkappa)} \begin{cases} G_1^{(-)}(x, y; W), & x > y, \\ G_1^{(+)}(x, y; W), & x < y. \end{cases}$$

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_1(x; W)\xi(x), \ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ and $\tilde{U} = v_1$. Therefore, the spectrum of $\hat{H}_1$ is simple.

The derivative of the spectral function is calculated via the function $M(c; W)$ using relations (5.22). The function M in this region is

$$M(c; W) = \frac{i\pi u_1(c; W) v_1(c; W)}{2k_0\Gamma(1+\varkappa)}.$$

Let $W = E = p^2 \geq 0$, $\beta = p = \sqrt{E} \geq 0$. Using the relation $H_\varkappa^{(1)}(px) = J_\varkappa(px) + iN_\varkappa(px)$ and the fact that $N_\varkappa(px)$ is real, we get

$$\sigma'(E) = \frac{\left(E/4k_0^2\right)^\varkappa}{2k_0\Gamma^2(1+\varkappa)}, \quad E \geq 0.$$

Let $W = E = -\tau^2 < 0$, $\tau = \sqrt{|E|} > 0$, $\beta = \mathrm{e}^{i\pi/2}\tau$. In this range of energies, we use the representations

$$u_1(x; E) = \Gamma(1+\varkappa)\,(\tau/2k_0)^{-\varkappa}\,(k_0x)^{1/2} I_\varkappa(\tau x),$$
$$v_1(x; E) = \frac{2}{i\pi}\,(\tau/2k_0)^{\varkappa}\,(k_0x)^{1/2} K_\varkappa(\tau x),$$

where $I_\varkappa(x)$ and $K_\varkappa(x)$ are Bessel functions of imaginary argument (see [1,20,81]), to obtain $\sigma'(E) = 0$, $E < 0$.

Thus, the simple spectrum of $\hat{H}_1$ is given by spec $\hat{H}_1 = \mathbb{R}_+$. The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}u_1(x; E) = \sqrt{\frac{x}{2}} J_\varkappa\left(\sqrt{E}x\right), \ E \geq 0, \tag{7.40}$$

of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. We note that in this case the corresponding inversion formulas coincide with the known formulas for the Fourier–Bessel transformation; see, for example, [7, 50].

7.2.4.2 The Second Region $-1/4 < \alpha < 3/4$

In this region, $0 < \varkappa < 1$ and there exists a one-parameter $U(1)$ family of s.a. Calogero Hamiltonians $\hat{H}_{2,\nu}$, $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, acting on the domains $D_{H_{2,\nu}}$ defined by (7.29).

For any $\alpha < 3/4$, the function $v_1(x; W)$ is square-integrable on $\mathbb{R}_+$, so that (7.39) can be rewritten as

$$\psi(x) = a_2 v_1(x; W) + \frac{i\pi}{2k_0 \Gamma(1+\varkappa)} u_1(x; W)\chi_\nu + Y(x),$$
$$\chi_\nu = \int_0^\infty v_1(y; W)\chi(y)\mathrm{d}y,\ Y(x) = \frac{i\pi}{2k_0\Gamma(1+\varkappa)} \int_0^x G_1^{(-)}(x, y; W)\,\chi(y)\mathrm{d}y$$
$$-\frac{i\pi}{2k_0\Gamma(1+\varkappa)} \int_0^x G_1^{(+)}(x, y; W)\chi(y)\mathrm{d}y. \tag{7.41}$$

Estimating the term $Y(x)$ with the help of the Cauchy–Schwarz inequality, we obtain

$$Y(x) = O(x^{3/2}),\ x \to 0, \tag{7.42}$$

which means that the asymptotic behavior of $\psi(x)$ as $x \to 0$ is due to the first two summands in (7.41). This allows one to find a_2 from the corresponding s.a. boundary conditions.

Using asymptotic formulas (7.37) and (7.38), we find that solution (7.41) satisfies s.a. boundary condition (7.28) if

$$a_2 = -\frac{\chi_\nu \pi^2 \cos\nu}{2k_0\Gamma(\varkappa)\Gamma(1+\varkappa)\omega_{2,\nu}(W)},\ \omega_\nu(W) = f(W)\cos\nu + \sin\nu,$$
$$f(W) = \frac{\Gamma(1-\varkappa)}{\Gamma(1+\varkappa)}\left(\mathrm{e}^{-i\pi/2}\beta/2k_0\right)^{2\varkappa}.$$

This implies that the Green's function of the Hamiltonian $\hat{H}_{2,\nu}$ reads

$$G(x, y; W) = \Omega(W)U_{2,\nu}(x; W)U_{2,\nu}(y; W)$$
$$-\frac{1}{2k_0\varkappa}\begin{cases} G^{(-)}(x, y; W),\ x > y, \\ G^{(+)}(x, y; W),\ x < y, \end{cases} \tag{7.43}$$

where

$$G^{(+)}(x, y; W) = U_{2,\nu}(x; W)\tilde{U}_{2,\nu}(y; W),$$
$$G^{(-)}(x, y; W) = \tilde{U}_{2,\nu}(x; W)U_{2,\nu}(y; W),$$
$$U_{2,\nu}(x; W) = u_1(x; W)\sin\nu + u_2(x; W)\cos\nu,$$
$$\tilde{U}_{2,\nu}(x; W) = u_1(x; W)\cos\nu - u_2(x; W)\sin\nu,$$
$$\Omega(W) = -\frac{\tilde{\omega}_{2,\nu}(W)}{2k_0\varkappa\omega_{2,\nu}(W)},\ \tilde{\omega}_\nu(W) = f(W)\sin\nu - \cos\nu,$$

and we used the relations

$$u_1(x; W) + \frac{i\pi}{\Gamma(\varkappa)\omega_{2,\nu}(W)}v_1(x; W) = \frac{U_{2,\nu}(x; W)}{\omega_\nu(W)},$$
$$v_1(x; W) = \frac{i\Gamma(\varkappa)}{\pi}\left[\tilde{\omega}_\nu(W)U_{2,\nu}(x; W) + \omega_\nu(W)\tilde{U}_{2,\nu}(x; W)\right].$$

We note that $U_{2,\nu}(x; W)$ and $\tilde{U}_{2,\nu}(x; W)$ are solutions of (7.36) real entire in W; $U_{2,\nu}(x; W)$ obeys the boundary condition (7.28), and the second summand on the right-hand side of (7.43) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x U_{2,\nu}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{2,\lambda}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{2,\nu}$ and $\tilde{U} = \tilde{U}_{2,\nu}$. Therefore, the spectra of $\hat{H}_{2,\lambda}$ are simple.

The spectral function is calculated via the function

$$M(c; W) = i\pi\omega_\nu^{-1}(W)G^{(+)}(c, c; W).$$

Thus, we obtain $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega(E + i0)$.

Let $W = E \geq 0$, $\beta = p = \sqrt{E} \geq 0$. We obtain

$$\sigma'(E) = \frac{\left(E/4k_0^2\right)^\varkappa}{2k_0\Gamma^2(1+\varkappa)\left[q^2 + q\cos(\pi\varkappa)\sin(2\nu) + \sin^2\nu\right]},$$
$$\sigma'(E) > 0,\ E > 0,\ q = \frac{\Gamma(1-\varkappa)}{\Gamma(1+\varkappa)}\left(E/4k_0^2\right)^\varkappa,$$

$\sigma'(0) = 0$ for $\nu \neq 0$, and $\sigma'(E)$ has an integrable singularity of the type $O(E^{-\varkappa})$ for $\nu = 0$.

Let $W = E = -\tau^2 < 0$, $\tau = \sqrt{|E|} > 0$, $\mathrm{e}^{-i\pi/2}\beta = \tau$. In this energy region, we find that if $\nu \in [0, \pi/2]$ or $\nu = -\pi/2$ then $\Omega(E)$ is finite and real and consequently $\sigma'(E) = 0$.

Let $\nu \in (-\pi/2, 0)$. Then we have

$$\sigma'(E) = \frac{\operatorname{Im} f_\nu^{-1}(E + i0)}{2\pi k_0 \varkappa \cos^2 \nu}, \;\; f_\nu(W) = f(W) - \tan|\nu|. \tag{7.44}$$

Since $f_\nu(E)$ is a real function, the left-hand side of (7.44) can differ from zero only at the points E that are negative roots of the equation $f_\nu(E) = 0$. For any fixed $\nu \in (-\pi/2, 0)$, the equation $f_\nu(E) = 0$ has only one negative solution,

$$E\,(\nu) = -4k_0^2 \left| \frac{\Gamma(1+\varkappa)}{\Gamma(1-\varkappa)} \tan|\nu| \right|^{1/\varkappa}. \tag{7.45}$$

According to Lemma 5.17, we obtain

$$\sigma'(E) = Q_\nu^2 \delta(E - E\,(\nu)),$$
$$Q_\nu = \frac{\left(|E\,(\nu)\,|/4k_0^2\right)^{-\varkappa/2}}{\varkappa \cos\nu} \sqrt{\frac{|E\,(\nu)\,|\Gamma(1+\varkappa)}{2k_0\Gamma(1-\varkappa)}}, \;\; E < 0. \tag{7.46}$$

Thus, for $\nu \in [0, \pi/2]$ or $\nu = -\pi/2$, the simple continuous spectrum of $\hat{H}_{2,\nu}$ is given by $\operatorname{spec} \hat{H}_{2,\nu} = \mathbb{R}_+$. The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}\,U_{2,\nu}(x; E), \;\; E \ge 0, \tag{7.47}$$

of $\hat{H}_{2,\nu}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $\nu \in (-\pi/2, 0)$, the spectrum of any s.a. Calogero Hamiltonian $\hat{H}_{2,\nu}$ is simple, and in addition to the nonnegative continuous spectrum, here there exists one negative level (7.45). Thus, $\operatorname{spec} \hat{H}_{2,\nu} = \mathbb{R}_+ \cup \{E\,(\nu)\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of generalized eigenfunctions (7.47) and one function

$$U(x) = Q_\nu U_{2,\nu}(x; E\,(\nu)) = \sqrt{\frac{2x|E\,(\nu)\,|\sin(\pi\varkappa)}{\pi\varkappa}} K_\varkappa \left(\sqrt{|E\,(\nu)\,|}x\right).$$

We note that the second region under consideration contains the point $\alpha = 0$ ($\varkappa = 1/2$), which represents the free-particle case. One can easily see that all the results obtained in Chap. 6 match the above consideration at $\alpha = 0$.

7.2.4.3 The Third Region $\alpha = -1/4$

In this region there exists a one-parameter $U(1)$ family of s.a. Calogero Hamiltonians $\hat{H}_{3,\nu}$, $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, acting on the domains $D_{H_{3,\nu}}$ (7.32).

In the case under consideration, formulas (7.41) and (7.42) hold. This allows one to find the constant a_2 from the boundary conditions (7.31),

$$a_2 = -\frac{\pi^2 \cos\nu}{4k_0\omega_\nu(W)},\ \omega_\nu(W) = f(W)\cos\nu - \sin\nu,$$
$$f(W) = \ln(\beta/2k_0) + \mathbf{C} - i\pi/2,$$

which implies that the Green's function of the s.a. Hamiltonian $\hat{H}_{3,\nu}$ is

$$G(x, y; W) = \Omega(W)U_{3,\nu}(x; W)U_{3,\nu}(x; W) + \frac{1}{k_0}\begin{cases} G^{(-)}(x, y; W),\ x > y, \\ G^{(+)}(x, y; W),\ x < y, \end{cases} \tag{7.48}$$

where

$$G^{(+)}(x, y; W) = U_{3,\nu}(x; W)\tilde{U}_{3,\nu}(y; W),$$
$$G^{(-)}(x, y; W) = \tilde{U}_{3,\nu}(x; W)U_{3,\nu}(y; W),$$
$$\Omega(W) = \frac{\tilde{\omega}_\nu(W)}{k_0\omega_\nu(W)},\ \tilde{\omega}_\nu(W) = f(W)\sin\nu + \cos\nu,$$
$$U_{3,\nu}(x; W) = u_1(x; W)\sin\nu + u_3(x; W)\cos\nu,$$
$$\tilde{U}_{3,\nu}(y; W) = u_1(x; W)\cos\nu - u_3(x; W)\sin\nu,$$
$$u_1(x; W) = (k_0x)^{1/2}J_0(\beta x),\ u_3(x; W) = \partial_\varkappa\left[u_1(x; W)|_{\varkappa\neq 0}\right]_{\varkappa=0},$$
$$v_1(x; W) = (k_0x)^{1/2}H_0^{(1)}(\beta x),$$
$$u_3(x; W) = (k_0x)^{1/2}\ln(k_0x)\,\tilde{O}(x^2),\ x \to 0,$$

and we used the relations

$$u_1(x; W) + \frac{i\pi\cos\nu}{2\omega_\nu(W)}v_1(x; W) = \frac{U_{3,\nu}(x; W)}{\omega_\nu(W)},$$
$$\pi v_1(x; W)/2i = \tilde{\omega}_\nu(W)U_{3,\nu}(x; W) + \omega_\nu(W)\tilde{U}_{3,\nu}(y; W).$$

We note that $U_{3,\nu}(x; W)$ and $\tilde{U}_{3,\nu}(x; W)$ are solutions of (7.36) real-entire in W; $U_{3,\nu}(x; W)$ obeys s.a. boundary condition (7.31), and the second summand on the right-hand side of (7.48) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x U_{3,\nu}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{3,\lambda}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{3,\nu}$ and $\tilde{U} = \tilde{U}_{3,\nu}$. Therefore, the spectra of $\hat{H}_{3,\nu}$ are simple.

The derivative of the spectral function is calculated via the function $M(c; W) = G(c, c; W)$, so that we have $\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega(E + i0)$.

Let $W = E \geq 0$, $\beta = p = \sqrt{E} \geq 0$. We obtain

$$\sigma'(E) = \left\{2k_0 \left([(\ln(p/2k_0) + \mathbf{C}) \cos\nu - \sin\nu]^2 + (\pi^2/4)\cos^2\nu \right)\right\}^{-1}.$$

Let $W = E < 0$, $\tau = \sqrt{|E|} > 0$, $\mathrm{e}^{-i\pi/2}\beta = \tau$. In this energy region, we have

$$\sigma'(E) = \frac{f(E)\sin\nu + \cos\nu}{f(E)\cos\nu - \sin\nu},\ f(E) = \ln(\tau/2k_0) + \mathbf{C}.$$

Let $\nu = \pm\pi/2$. In this case $\Omega(E) = -f(E)/k_0$ is a finite and real function such that we obtain $\sigma'(E) = 0$.

Let $|\nu| < \pi/2$. Then we have

$$\sigma'(E) = \frac{\operatorname{Im} f_\nu^{-1}(E + i0)}{\pi k_0 \cos^2\nu},\ f_\nu(W) = f(W) - \tan\nu. \tag{7.49}$$

Since $f_\nu(E)$ is a real function, the left-hand side of (7.49) can differ from zero only at the points E that are negative roots of the equation $f_\nu(E) = 0$. For any fixed $\nu \in (-\pi/2, \pi/2)$, the equation $f_\nu(E) = 0$ has only one negative solution,

$$E(\nu) = -4k_0^2 \exp(2\tan\nu - 2\mathbf{C}).$$

According to Lemma 5.17, we obtain the right-hand side of (7.49),

$$\sigma'(E) = Q_\nu^2 \delta(E - E(\nu)),\ Q_\nu = \frac{1}{\cos\nu}\sqrt{\frac{2|E(\nu)|}{k_0}}\ E < 0.$$

Thus, for $\nu = \pm\pi/2$, the simple continuous spectrum of $\hat{H}_{3,\nu}$ is given by $\operatorname{spec} \hat{H}_{3,\pm\pi/2} = \mathbb{R}_+$.

The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}u_1(x; E) = \sqrt{x/2}J_0\left(\sqrt{E}x\right),\ E \geq 0,$$

of $\hat{H}_{3,\pm\pi/2}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $\nu \in (-\pi/2, \pi/2)$, the spectrum of any s.a. Calogero Hamiltonian $\hat{H}_{3,\nu}$, is simple, and in addition to the nonnegative continuous spectrum, here there exists one negative level (7.45). Thus, spec $\hat{H}_{3,\nu} = \mathbb{R}_+ \cup \{E(\nu)\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of generalized eigenfunctions $U_E(x)$ of the continuous spectrum,

$$U_E(x) = \sqrt{\sigma'(E)}U_{3,\nu}(x;E),\ E \geq 0,$$

and one function $U(x)$ of the discrete spectrum,

$$U(x) = -Q_\nu U_{3,\nu}(x;E(\nu)) = \sqrt{2|E(\lambda)|x}K_0\left(\sqrt{|E(\lambda)|x}\right).$$

7.2.4.4 The Fourth Region $\alpha < -1/4$

In this region $\varkappa = i\sigma$ and there exists a one-parameter $U(1)$ family of s.a. Calogero Hamiltonians $\hat{H}_{4,\theta}$, $\theta \in \mathbb{S}(0,\pi)$, specified by their domains (7.34).

In the case under consideration $\varkappa = i\sigma$, $\sigma > 0$, and formulas (7.41) and (7.42) hold. This allows one to find the constant a_2 from the boundary conditions (7.33),

$$a_2 = -\frac{\pi\sin(i\sigma)\mathrm{e}^{-i\tilde{\theta}}}{2k_0\omega_\theta(W)},\ \omega_\theta(W) = \mathrm{e}^{-i\tilde{\theta}}\left(\mathrm{e}^{-i\pi/2}\beta/2k_0\right)^{2i\sigma} + \mathrm{e}^{i\tilde{\theta}},$$
$$\tilde{\theta} = \theta + \theta_\Gamma,\ \theta_\Gamma = \frac{1}{2i}\ln\frac{\Gamma(1+i\sigma)}{\Gamma(1-i\sigma)}.$$

This implies that the Green's function of s.a. Hamiltonian $\hat{H}_{4,\theta}$ reads

$$G(x,y;W) = \Omega(W)U_{4,\theta}(x;W)U_{4,\theta}(y;W) - \frac{1}{4k_0\sigma}\begin{cases} G^{(-)}(x,y;W),\ x>y, \\ G^{(+)}(x,y;W),\ x<y, \end{cases} \tag{7.50}$$

where

$$G^{(+)}(x,y;W) = U_{4,\theta}(x;W)\tilde{U}_{4,\theta}(y;W),\ \Omega(W) = \frac{i}{4k_0\sigma}\frac{\tilde{\omega}_{4,\theta}(W)}{\omega_{4,\theta}(W)},$$
$$G^{(-)}(x,y;W) = \tilde{U}_{4,\theta}(x;W)U_{4,\theta}(y;W),$$
$$U_{4,\theta}(x;W) = \mathrm{e}^{i\theta}u_1(x;W) + \mathrm{e}^{-i\theta}u_2(x;W),$$
$$\tilde{U}_{4,\theta}(x;W) = -i\left[\mathrm{e}^{i\theta}u_1(x;W) - \mathrm{e}^{-i\theta}u_2(x;W)\right],$$
$$\tilde{\omega}_\theta(W) = \mathrm{e}^{-i\tilde{\theta}}\left(\mathrm{e}^{-i\pi/2}\beta/2k_0\right)^{2i\sigma} - \mathrm{e}^{i\tilde{\theta}},$$

and we used the relations

$$u_1(x;W) + \frac{\sin(i\pi\sigma)e^{-i\tilde{\theta}}\Gamma(1+i\sigma)}{\omega_\theta(W)}v_1(x;W) = \frac{e^{i\theta_\Gamma}}{\omega_\theta(W)}U_{4,\theta}(x;W),$$

$$v_1(x;W) = \frac{e^{-i\theta_\Gamma}\Gamma(i\sigma)}{2\pi}\left[i\tilde{\omega}_\theta(W)U_{4,\theta}(x;W) - \omega_\theta(W)\tilde{U}_{4,\theta}(x;W)\right].$$

We note that $U_{4,\theta}(x;W)$ and $\tilde{U}_{4,\theta}(x;W)$ are solutions of (7.36), real entire in W; $U_{4,\theta}(x;W)$ satisfies the boundary conditions (7.33), and the second summand in the right-hand side of (7.50) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty dx U_{4,\theta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{4,\theta}}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{4,\theta}$ and $\tilde{U} = \tilde{U}_{4,\theta}$. Therefore, the spectra of $\hat{H}_{4,\theta}$ are simple.

The derivative of the spectral function is calculated via the function $M(c;W) = G(c,c;W)$, so that we have $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega(E+i0)$.

For $E \geq 0$, we obtain

$$\sigma'(E) = \frac{(4\pi k_0\sigma)^{-1}\sin h(\pi\sigma)}{\cos h(\pi\sigma) + \cos\Phi(E)},\quad \Phi(E) = \sigma\ln(E/4k_0^2) - 2\tilde{\theta}. \tag{7.51}$$

Let $W = E < 0$. In this energy region the function $\Omega(E)$ is real, $\Omega(E) = -[2k_0\sigma\cot[\Phi(E)]$, $\Phi(E) = \sigma\ln(\tau/2k_0) - \tilde{\theta}$, so that $\sigma'(E)$ can differ from zero only at the points $E_n(\theta)$ where $\cot[\Phi(E_n(\theta))] = 0$. These points are

$$E_n(\theta) = -4k_0^2 e^{2\left(\pi/2+\pi n+\tilde{\theta}\right)/\sigma},\ n \in \mathbb{Z}.$$

Using considerations similar to what we used to derive (7.46), we obtain

$$\sigma'(E) = \sum_{n\in\mathbb{Z}} Q_n^2\delta(E - E_n(\theta)),\ Q_n = \frac{1}{\sigma}\sqrt{\frac{|E_n(\theta)|}{2k_0}},\ E_n(\theta) < 0. \tag{7.52}$$

Equations (7.51) and (7.52) imply that the simple spectrum of $\hat{H}_{4,\theta}$ reads spec $\hat{H}_{4,\theta} = \mathbb{R}_+ \cup \{E_n(\theta),\ n \in \mathbb{Z}\}$. A complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of the generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}U_{4,\theta}(x;E),\ E \geq 0,$$

and of the eigenfunctions $U_n(x)$, $n \in \mathbb{Z}$,

$$U_n(x) = iQ_n U_{4,\theta}(x; E_n(\theta)) = \sqrt{\frac{2x|E_n(\theta)|\sin h(\pi\sigma)}{\pi\sigma}} K_{i\sigma}(|E_n(\theta)|^{1/2}x),$$

of the discrete negative part of the spectrum. We see that the discrete spectrum is unbounded from below and has an accumulation point in zero energy.

7.2.5 The Fate of Scale Symmetry

The scale parameter k_0, introduced for dimensional reasons, appears to be significant in s.a. extensions for $\alpha < 3/4$: its change $k_0 \to lk_0$ generally changes the extension parameter, which indicates the breaking of scale symmetry.

From the mathematical standpoint, it is convenient to parameterize s.a. extensions by a dimensionless parameter, ν or θ. However, from the physical standpoint, it seems more appropriate to convert the two parameters, the fixed dimensional parameter k_0 of spatial dimension $\mathrm{d}_{k_0} = -1$ and the varying dimensionless parameters ν and θ, to a one-dimensional parameter μ of spatial dimension $\mathrm{d}_\mu = -1$ uniquely parameterizing the extensions, and the parameter k_0 no longer enters the description. This makes evident the spontaneous breaking of the scale symmetry.

As is easily seen from (7.28), in the case of $-1/4 < \alpha < 3/4$ and for $\nu \in (0, \pi/2)$, this parameter is $\mu = k_0(\tan\nu)^{1/2\varkappa}$, $0 < \mu < \infty$. The s.a. Calogero Hamiltonian $\hat{H}_{2,\nu}$ with $\nu \in (0, \pi/2)$ is now naturally labeled by the subscript μ and an extra subscript $+$ indicating the sign of ν, $\hat{H}_{2,\mu,+} = \hat{H}_{2,\nu}$, $\nu \in (0, \pi/2)$, and is specified by the a.b. conditions at the origin,

$$\begin{aligned}
\psi_{\mu,+}(x) &= Cx^{1/2}\left[(\mu x)^\varkappa + (\mu x)^{-\varkappa}\right] + O(x^{3/2}),\\
\psi'_{\mu,+}(x) &= Cx^{-1/2}\left[(1/2+\varkappa)(\mu x)^\varkappa + (1/2-\varkappa)(\mu x)^{-\varkappa}\right] + O(x^{1/2}).
\end{aligned} \tag{7.53}$$

The complete orthonormalized system (7.47) of eigenfunctions for the Hamiltonian $\hat{H}_{2,\mu,+}$ is presented in terms of the scale parameter μ as follows:

$$\begin{aligned}
U_E(x) &= \sqrt{\frac{x}{2}} \frac{J_\varkappa(\sqrt{E}x) + \gamma(\mu, E) J_{-\varkappa}(\sqrt{E}x)}{\sqrt{1 + 2\gamma(\mu, E)\cos\pi\varkappa + \gamma^2(\mu, E)}},\\
\gamma(\mu, E) &= \frac{\Gamma(1-\varkappa)}{\Gamma(1+\varkappa)}\left(E/4\mu^2\right)^\varkappa, \quad E \geq 0;
\end{aligned} \tag{7.54}$$

the auxiliary scale parameter k_0 then disappears.

For $\nu \in (-\pi/2, 0)$, the dimensional parameter is $\mu = k_0|\tan\nu|^{1/2\varkappa}$, $0 < \mu < \infty$. The Hamiltonian $\hat{H}_{2,\nu}$ with $\nu \in (-\pi/2, 0)$ is now denoted by $\hat{H}_{2,\mu,-}$:

$\hat{H}_{2,\mu,-} = \hat{H}_{2,\nu},\ \nu \in (-\pi/2, 0)$, and is specified by the a.b. conditions at the origin,

$$\psi_{\mu,-}(x) = Cx^{1/2}\left[(\mu x)^{\varkappa} - (\mu x)^{-\varkappa}\right] + O(x^{3/2}),$$
$$\psi'_{\mu,-}(x) = Cx^{-1/2}\left[(1/2+\varkappa)(\mu x)^{\varkappa} - (1/2-\varkappa)(\mu x)^{-\varkappa}\right] + O(x^{1/2}). \quad (7.55)$$

The single negative energy level representing its discrete spectrum is now given by

$$E_{\mu,-} = -4\mu^2 \left(\frac{\Gamma(1+\varkappa)}{\Gamma(1-\varkappa)}\right)^{1/\varkappa}. \quad (7.56)$$

The complete orthonormalized system of eigenfunctions for the Hamiltonian $\hat{H}_{2,\mu,-}$, written in terms of the scale parameter μ, consists of the functions (7.55) and one additional function

$$U(x) = \sqrt{\frac{2x\left|E_{\mu,-}\right|\sin\pi\varkappa}{\pi\varkappa}}\,K_{\varkappa}\left(\sqrt{\left|E_{\mu,-}\right|}x\right). \quad (7.57)$$

We note that the s.a. Calogero Hamiltonian $\hat{H}_{2,\mu,-}$ is uniquely determined by the position of the negative energy level.

The exceptional values $\nu = 0$ and $|\nu| = \pi/2$ of the extension parameter are naturally included in this scheme as the respective exceptional values $\mu = 0$ and $\mu = \infty$ of the scale parameter, and in terms of μ the corresponding Hamiltonians are respectively denoted by $\hat{H}_{2,0} = \hat{H}_{2,\mu=0} = \hat{H}_{2,\nu=0}$ and $\hat{H}_{2,\infty} = \hat{H}_{2,\mu=\infty} = \hat{H}_{2,|\nu|=\pi/2}$.

As can be seen from (7.31), in the case of $\alpha = -1/4$ and for $|\nu| < \pi/2$, the dimensional parameter is $\mu = k_0 e^{\tan\nu},\ 0 < \mu < \infty$. In terms of μ, the respective s.a. Calogero Hamiltonian $\hat{H}_{3,\mu}$, $\hat{H}_{3,\mu} = \hat{H}_{3,\nu}$, is specified by a.b. conditions at the origin,

$$\psi_{\mu}(x) = Cx^{1/2}\ln(\mu x) + O(x^{3/2}),$$
$$\psi'_{\mu}(x) = Cx^{-1/2}\left[\frac{1}{2}\ln(\mu x) + 1\right] + O(x^{1/2}). \quad (7.58)$$

The single negative energy level representing its discrete spectrum is given by $E_{\mu} = -4\mu^2\exp(-2\mathbf{C})$; the position of this level uniquely determines the Hamiltonian $\hat{H}_{3,\mu}$.

The exceptional values $\lambda = \pi/2 \sim \lambda = -\pi/2$ of the extension parameter ν are naturally included as the respective exceptional values $\mu = \infty \sim \mu = 0$ of the scale parameter μ. In terms of μ, we let $\hat{H}_3$ denote the corresponding Hamiltonian, $\hat{H}_3 = \hat{H}_{3,|\nu|=\pi/2}$.

As is seen from (7.33), in the case of $\alpha < -1/4$, the dimensional parameter is

$$\mu = k_0 \mathrm{e}^{\theta/\sigma},\ \mu_0 \leq \mu \leq \mu_0\, \mathrm{e}^{\pi/\sigma},\ \mu_0 \sim \mu_0 \mathrm{e}^{\pi/\sigma} \tag{7.59}$$

with some fixed $\mu_0 > 0$. In terms of μ, the respective s.a. Calogero Hamiltonian $\hat{H}_{4,\mu}$, $\hat{H}_{4,\mu} = \hat{H}_{4,\theta}$, is specified by a.b. conditions at the origin,

$$\begin{aligned} \psi_\mu(x) &= C x^{1/2}\left[(\mu x)^{i\sigma} + (\mu x)^{-i\sigma}\right] + O(x^{3/2}), \\ \psi'_\mu(x) &= C x^{-1/2}\left[(1/2 + i\sigma)(\mu x)^{i\sigma} - (1/2 - i\sigma)(\mu x)^{-i\sigma}\right] + O(x^{1/2}). \end{aligned} \tag{7.60}$$

The infinite sequence of negative energy levels representing its discrete spectrum is given by

$$E_{\mu,n} = -4\mu^2 \exp\frac{\pi + \theta_\sigma + 2\pi n}{\sigma},\ \ \theta_\sigma = -i \ln\frac{\Gamma(1 + i\sigma)}{\Gamma(1 - i\sigma)},\ n \in \mathbb{Z}; \tag{7.61}$$

the position of one of negative energy levels in any of the intervals

$$\left(-4\mu_0^2 \mathrm{e}^{\frac{\theta_\sigma + \pi + 2\pi m}{\sigma}},\ -4\mu_0^2 \mathrm{e}^{\frac{\theta_\sigma - \pi + 2\pi m}{\sigma}}\right),\ \ m \in \mathbb{Z},$$

uniquely determines the Hamiltonian $\hat{H}_{4,\mu}$. The complete orthonormalized system of eigenfunctions for the Hamiltonian $\hat{H}_{4,\mu}$ is written in terms of the scale parameter μ as follows:

$$\begin{aligned} U_E(x) &= \sqrt{\frac{x/4}{\cos h\pi\sigma + \cos \Phi_\mu(E)}}\left[\varphi_\mu(E)\left(E/4\mu^2\right)^{-i\sigma/2} J_{i\sigma}\left(\sqrt{E}x\right)\right. \\ &\quad \left. + \varphi_\mu^{-1}(E)\, J_{-i\sigma}\left(\sqrt{E}x\right)\right], \\ \Phi_\mu(E) &= \sigma \ln(E/4\mu^2) - \theta_\sigma,\ \ \varphi_\mu(E) = \mathrm{e}^{i\theta_\sigma/2}\left(E/4\mu^2\right)^{-i\sigma/2},\ \ E \geq 0; \\ U_n(x) &= \sqrt{\frac{2x|E_{\mu,n}| \sin h\pi\sigma}{\pi\sigma}}\, K_{i\sigma}\left(\sqrt{|E_{\mu,n}|}x\right),\ n \in \mathbb{Z}. \end{aligned} \tag{7.62}$$

The scale parameter μ, as well as μ_0, is evidently defined modulo the factor $\exp \pi m/\sigma$, $m \in \mathbb{Z}$; the a.b. conditions (7.60) are invariant under the change $\mu \to \mathrm{e}^{\pi m/\sigma}\mu$; accordingly, the discrete spectrum (7.61) is also invariant under this change, and the same holds for the normalized eigenfunctions (7.62) up to the irrelevant factor -1 in front of eigenfunctions of continuous spectrum for odd m.

All s.a. Calogero Hamiltonians that form a $U(1)$ family for each value of the coupling constant α in all three regions of the values of $\alpha < 3/4$ are thus parameterized by a scale parameter μ, and in the region $-1/4 < \alpha < 3/4$ we must distinguish two different subfamilies by an additional index $+$ or $-$.

We now turn to the problem of the scale symmetry for s.a. Calogero Hamiltonians. The scale symmetry is associated with the one-parameter group of unitary scale transformations $\hat{U}(l)$, $l > 0$, defined by (7.18). Under a preliminary "naïve" treatment of the Calogero problem, see Sect. 7.2.2, the "naïve" Hamiltonian $\hat{H}$ identified with the initial differential expression (7.16), which has been considered an s.a. operator without any reservations about its domain, formally satisfies the scale symmetry relation (7.19). It is this relation that is a source of "paradoxes" concerning the spectrum of the "naïve" $\hat{H}$. Below, we resolve these paradoxes.

If we extend relation (7.19) to the s.a. Calogero Hamiltonians $\hat{H}_{[i]}$, $[i] = 1; 2, \mu, +; 2, \mu, -; 3, \mu; 4, \mu$, we must recognize that this relation is nontrivial because the operators $\hat{H}_{[i]}$ are unbounded, and in general, their domains $D_{H_{[i]}}$ change with changing the scale parameter μ that naturally changes under scale transformations. The relation

$$\hat{U}^{-1}(l)\,\hat{H}_{[i]}\hat{U}(l) = l^{-2}\hat{H}_{[i]} \Longleftrightarrow \hat{H}_{[i]}\hat{U}(l) = l^{-2}\hat{U}(l)\,\hat{H}_{[i]} \tag{7.63}$$

for the Hamiltonian $\hat{H}_{[i]}$ with a specific $[i]$, if it holds, implies that apart from the fact that "the rule of action" of the operator $\hat{H}_{[i]}$ changes in accordance with (7.63), its domain $D_{H_{[i]}}$ is invariant under scale transformations:

$$\hat{U}(l)D_{H_{[i]}} = D_{H_{[i]}}. \tag{7.64}$$

In such a case, we say that the Hamiltonian $\hat{H}_{[i]}$ is scale-covariant and is of scale dimension $\mathrm{d}_{H_{[i]}} = -2$; in short, we speak about the scale symmetry of the Hamiltonian $\hat{H}_{[i]}$. If relation (7.64) does not hold, i.e., if the domain $D_{H_{[i]}}$ of the Hamiltonian $\hat{H}_{[i]}$ is not scale-invariant, we are forced to speak about the phenomenon of a spontaneous breaking of scale symmetry for the Hamiltonian $\hat{H}_{[i]}$.

The initial symmetric operator $\hat{H}$ and its adjoint $\hat{H}^+$ associated with the differential expression (7.16) are scale-covariant because both $D_H = \mathcal{D}(\mathbb{R}_+)$ and $D_{H^+} = D^*_{\check{H}}(\mathbb{R}_+)$ are evidently scale-invariant. The s.a. extensions $\hat{H}_{[i]}$ of the scale-covariant $\hat{H}$ can lose this property. On the other hand, $\hat{H}_{[i]}$ are s.a. restrictions of $\hat{H}^+$, and their domains $D_{H_{[i]}}$ belong to the scale-invariant domain D_{H^+}, $D_{H_{[i]}} \subseteq D_{H^+}$. Therefore, the scale symmetry of a specific Hamiltonian $\hat{H}_{[i]}$ is determined by the behavior of the a.b. conditions specifying this s.a. operator and thus restricting its domain in comparison with D_{H^+} under scale transformations. This behavior is different for different $[i]$; namely, it is different for the above four regions of the values of α (see Sect. 7.2.3) and strongly depends on the value of the scale parameter μ specifying the s.a. Hamiltonians in each of the last three regions. We consider these four regions sequentially.

(i) First region: $\alpha \geq 3/4$.

For each α in this region, the single s.a. Calogero Hamiltonian $\hat{H}_1$ coincides with the operator $\hat{H}^+$, $\hat{H}_1 = \hat{H}^+$, and is therefore scale-covariant,

$$\hat{U}\,(l)\,\hat{H}_1\hat{U}^{-1}(l) = l^{-2}\hat{H}_1. \tag{7.65}$$

In other words, the scale symmetry holds for $\alpha \geq 3/4$. The scale transformation law (7.18) as applied to eigenfunctions (7.40) yields

$$U_E(x) \longmapsto \hat{U}\,(l)\,U_E(x) = l^{-1}U_{l^{-2}E}(x), \tag{7.66}$$

which we treat, in particular, as the scale transformation law for the energy spectrum, given by

$$E \longmapsto l^{-2}E, \tag{7.67}$$

i.e., the spatial dimension of energy $\mathrm{d}_E = -2$. The group of scale transformations acts transitively on the energy spectrum, the semiaxis $\mathbb{R}_+$, except the point $E = 0$, which is a stationary point. This coincides with our preliminary expectations in Sect. 7.2.2.

(ii) Second region: $-1/4 < \alpha < 3/4$.

The change of a.b. conditions (7.53) under scale transformations (7.18) is given by the natural scale transformation

$$\mu \longmapsto l^{-1}\mu \tag{7.68}$$

of the dimensional scale parameter μ (its spatial dimension being -1), or, in terms of the dimensionless extension parameter λ, by

$$\tan\nu \longmapsto l^{-2\varkappa}\tan\nu, \tag{7.69}$$

which implies that under the scale transformations the respective domain $D_{H_{2,\mu,+}}$ of the Hamiltonian $\hat{H}_{2,\mu,+}$ transforms to $D_{H_{2,l^{-1}\mu,+}}$,

$$D_{H_{2,\mu,+}} \longmapsto \hat{U}(l)D_{H_{2,\mu,+}} = D_{H_{2,l^{-1}\mu,+}}\,. \tag{7.70}$$

It follows that the scale transformations change the Hamiltonian $\hat{H}_{2,\mu,+}$ to another Hamiltonian $\hat{H}_{2,l^{-1}\mu,+}$,

$$\hat{H}_{2,\mu,+} \longmapsto \hat{U}\,(l)\,\hat{H}_{2,\mu,+}\hat{U}^{-1}(l) = l^{-2}\hat{H}_{2,l^{-1}\mu,+}, \tag{7.71}$$

which means that the scale symmetry is spontaneously broken for the Hamiltonians $\hat{H}_{2,\mu,+}$. The scale transformation law for the eigenfunctions (7.54) is given by

$$U_E(x) \longmapsto \hat{U}(l)\,U_E(x) = l^{-1}U_{l^{-2}E}(x)\big|_{\mu\longmapsto l^{-1}\mu} . \tag{7.72}$$

The same evidently holds for the Hamiltonians $\hat{H}_{2,\mu,-}$ specified by a.b. conditions (7.55): the respective formulas (7.68) and (7.69) remain unchanged, while in formulas (7.70), (7.71), and (7.72) the subscript $+$ changes to the subscript $-$, and formula (7.72) for the eigenfunctions of the continuous spectrum is supplemented by the formula for the bound-state eigenfunction (7.57), (7.56),

$$U(x) \longmapsto \hat{U}(l)\,U(x) = U(x)|_{\mu\longmapsto l^{-1}\mu}\,,\ \ E_{l^{-1}\mu,-} = l^{-2}E_{\mu,-}\,. \tag{7.73}$$

The Hamiltonians $\hat{H}_{2,\infty}$ and $\hat{H}_{2,0}$ corresponding to the respective exceptional values $\mu = \infty\,(|\nu| = \pi/2)$ and $\mu = 0\,(\lambda = 0)$ and specified by the respective a.b. conditions

$$\psi(x) = Cx^{1/2+\varkappa} + O(x^{3/2}),\ x \to 0;\ \ \psi(x) = Cx^{1/2-\varkappa} + O(x^{3/2}),\ x \to 0,$$

are scale-covariant, which means that copies of formulas (7.65), (7.66), and (7.67) with subscript 1 replaced by the respective subscripts $2,\infty$ and $2,0$ hold. If we require scale symmetry in the Calogero problem, then only the two possibilities $\hat{H}_{2,\infty}$ and $\hat{H}_{2,0}$ remain for the s.a. Calogero Hamiltonian in the interval $-1/4 < \alpha < 3/4$.

We note that this interval of α includes the point $\alpha = 0$ corresponding to a free motion. Therefore, all we have said concerning the spontaneous scale-symmetry breaking relates to the case of a free particle on a semiaxis.

(iii) Third region: $\alpha = -1/4$.

The change of the a.b. conditions (7.58) under the scale transformations (7.18) is equivalent to rescaling (7.68) the dimensional parameter μ, or to the change $\tan\nu \to \tan\nu - \ln l$ of the dimensionless extension parameter ν. A further consideration is completely similar to the preceding one, to yield that copies of relations (7.70), (7.71), (7.72), and (7.73), with the subscript 2 replaced by the subscript 3, and with the subscripts $+$ and $-$ eliminated, hold for the Hamiltonians $\hat{H}_{3,\mu}$, which implies scale-symmetry breaking for these Hamiltonians.

Regarding the Hamiltonian $\hat{H}_3$ corresponding to the exceptional values $\mu = 0$ and $\mu = \infty$ of the scale parameter μ, which are equivalent, $0 \sim \infty$, and specified by the a.b. conditions $\psi(x) = Cx^{1/2} + O(x^{3/2})$, this Hamiltonian is scale-covariant, and copies of relations (7.65), (7.66), and (7.67) with the substitution $1 \to 3$ hold. If we require scale symmetry for the s.a. Calogero Hamiltonian with $\alpha = -1/4$, then it is only the Hamiltonian $\hat{H}_3$ that survives.

(iv) Fourth region: $\alpha < -1/4$.

The change of the a.b. conditions (7.60) under the scale transformations (7.18) is equivalent to a modified rescaling $\mu \to l^{-1}\mu \exp \pi m/\sigma$ of the dimensional extension parameter μ, where an integer m is defined by the condition

$$\mu_0 \leq l^{-1}\mu \exp(\pi m/\sigma) < \mu_0 \exp(\pi/\sigma);$$

the changed μ must remain within the interval $[\mu_0, \mu_0 \exp \pi/\sigma)$, see (7.59); this is equivalent to the change $\theta \to (\theta + \sigma \ln l)|_{\mathrm{mod}\,\pi}$ of the dimensionless extension parameter θ. It follows that for the Hamiltonians $\hat{H}_{4,\mu}$, $\mu_0 \leq \mu \leq \mu_0 \mathrm{e}^{\pi/\sigma}$, $\mu_0 \sim \mu_0 \mathrm{e}^{\pi/\sigma}$, the relations

$$\begin{aligned}
&D_{H_{4,\mu}} \longmapsto \hat{U}(l) D_{H_{4,\mu}} = D_{H_{4,\mu l^{-1}\exp \pi m/\sigma}},\\
&\hat{H}_{4,\mu} \longmapsto \hat{U}(l)\, \hat{H}_{4,\mu} \hat{U}^{-1}(l) = l^{-2} \hat{H}_{4,\mu l^{-1}\exp \pi m/\sigma},\\
&U_n(x) \longmapsto \hat{U}(l)\, U_n(x) = U_n(x)|_{E_{\mu,n} \longmapsto E_{\mu l^{-1}\exp \pi m/\sigma, n-m}},\\
&E_{\mu l^{-1}\exp \pi m/\sigma, n-m} = l^{-2} E_{\mu,n},\\
&U_E(x) \longmapsto \hat{U}(l)\, U_E(x) = (-1)^m l^{-1}\, U_{l^{-2}E}(x)|_{\mu \longmapsto \mu l^{-1}\exp \pi m/\sigma}
\end{aligned}$$

hold.

This means that the scale symmetry is spontaneously broken for $\hat{H}_{4,\mu}$. The peculiar feature of the fourth region is that for $l = \exp \pi n/\sigma$, $n \in \mathbb{Z}$, the scale symmetry holds. In other words, the scale symmetry is not broken completely, but to up an infinite cyclic subgroup. In particular, this subgroup acts transitively on the discrete energy spectrum.

This is the fate of the scale symmetry in the QM Calogero problem.

The paradoxes concerning the scale symmetry in the Calogero problem and considered in Sect. 7.2.2 are thus resolved. Namely, in general, there is no scale symmetry in the problem for $\alpha < 3/4$. In the latter case, the "naïve" Calogero Hamiltonian $\hat{H}$ of Sect. 7.2.2 is actually the operator $\hat{H}^+$ that is scale-covariant but not s.a. As for s.a. Calogero Hamiltonians, all possibilities for a negative part of the energy spectrum considered in Sect. 7.2.2 are generally realized by different Hamiltonians specified by different a.b. conditions. In general, the scale symmetry shifts energy levels together with Hamiltonians.

We conclude the above consideration with the following remarks for physicists.

We have a unique QM description of a nonrelativistic particle moving on a semiaxis in the Calogero potential with the coupling constant $\alpha \geq 3/4$. In the case of $\alpha < 3/4$, mathematics presents different possibilities related to different admissible s.a. asymptotic boundary conditions at the origin that are specified in terms of the scale parameter μ. But a final choice, which is reduced to a specific choice of the scale parameter μ, belongs to the physicist.

The origin of this parameter presents a physical problem, as well as the physical interpretation of the chosen s.a. Hamiltonian, as a whole. We note only that the usual regularization (7.17) of the Calogero potential by a cutoff at a finite radius and the consequent passage to the limit of zero radius yields $\mu = \infty$ in the case of $-1/4 \leq \alpha < 3/4$; a peculiar feature of the case of $\alpha = -1/4$ is that $\mu = \infty$ is equivalent to $\mu = 0$. Such a choice of the scale parameter corresponds to the minimum possible singularity of wave functions in the s.a. Hamiltonian domain at the origin. In the case of $\alpha < -1/4$, the regularization procedure does not provide an answer: the zero-radius limit does not exist. A suggestion on the nature of the scale parameter μ, $0 \leq \mu < \infty$, in the case of $-1/4 < \alpha < 3/4$, $0 < \mu < \infty$ in the case of $\alpha = -1/4$, and $\mu_0 \leq \mu \leq \mu_0 \exp \pi/\sigma$ in the case of $\alpha < -1/4$, has been presented above in Sect. 7.2.3: it is conceivable that this parameter is a manifestation of an additional δ-like term in the potential.

In deciding on a specific value of the scale parameter μ, one of the additional arguments can be related to scale symmetry. In the case of $\alpha \geq 3/4$, scale symmetry holds. In the case of $-1/4 \leq \alpha < 3/4$, scale symmetry is spontaneously broken for a generic μ. As for any spontaneously broken symmetry, scale symmetry does not disappear but transforms one physical system to another inequivalent physical system. But if we require scale symmetry, as we do in similar situations with rotational symmetry or reflection symmetry, then a possible choice strongly narrows to $\mu = \infty$ (the minimum possible singularity of wave functions at the origin) or $\mu = 0$ (the maximum possible singularity) in the case of $-1/4 < \alpha < 3/4$ and to $\mu = \infty \sim \mu = 0$ (the minimum possible singularity) in the case of $\alpha = -1/4$. For strongly attractive Calogero potentials with $\alpha < -1/4$, the requirement of scale symmetry cannot be fulfilled: scale symmetry is spontaneously broken for any μ.

7.3 Schrödinger Operators with Potentials Localized at the Origin

7.3.1 *Self-adjoint Schrödinger Operators*

Let $V^\circ(x)$ be an arbitrary *potential localized at the origin*, and $\check{H}$ the corresponding differential operation,

$$\check{H} = \check{\mathcal{H}} + V^\circ(x) = -d_x^2 + V^\circ(x) .$$

Our aim is to study possible s.a. Schrödinger operators associated with this differential operation. Using additional physical considerations, one can identify some of them with specific forms of $V^\circ(x)$, namely, with a δ-potential field $V^\circ(x) = \delta(x)$.

As usual, we start with an initial symmetric operator $\hat{H}$ associated with $\check{H}$.

The first supposition is that the domain D_H of the initial symmetric operator $\hat{H}$ has the form

$$D_H = \mathcal{D}\left(\mathring{\mathbb{R}}\right) = \mathcal{D}(-\infty, 0) \cup \mathcal{D}(0, \infty), \quad \mathring{\mathbb{R}} = (-\infty, 0) \cup (0, \infty).$$

In other words, we believe that domains of any extensions of $\hat{H}$ must include all the functions from $\mathcal{D}\left(\mathring{\mathbb{R}}\right)$.

The subspace $\mathcal{D}\left(\mathring{\mathbb{R}}\right)$ is dense in $L^2(\mathbb{R})$, $\overline{\mathcal{D}\left(\mathring{\mathbb{R}}\right)} = L^2(\mathbb{R})$. All the functions from $\mathcal{D}\left(\mathring{\mathbb{R}}\right)$ vanish both at infinity and in a neighborhood of the point $x = 0$ together with all their derivatives.

The second supposition, which seems to be quite natural, is that the operator $\hat{H}$ acts as $\check{\mathcal{H}} = -d_x^2$ on functions from $\mathcal{D}\left(\mathring{\mathbb{R}}\right)$ (i.e., $V^\circ(x)$ acts as the zero operator on such functions).

Thus, we choose the initial symmetric operator $\hat{H}$ as follows:

$$\hat{H} : \begin{cases} D_H = \mathcal{D}\left(\mathring{\mathbb{R}}\right), \\ \hat{H}\psi = \check{\mathcal{H}}\psi = -d_x^2\psi, \ \forall \psi \in \mathcal{D}\left(\mathring{\mathbb{R}}\right). \end{cases} \tag{7.74}$$

The symmetry of the operator (7.74) is obvious.

The next step is standard. One needs to calculate the adjoint $\hat{H}^+$ to $\hat{H}$. Following the general considerations of Chap. 4, we first construct the operator $\hat{H}^*$, which in the case under consideration, we define as

$$\hat{H}^* : \begin{cases} D_{H^*}(\mathbb{R}) = D^*_{\check{H}}(\mathbb{R}) = \left\{\psi_* : \psi_*, \psi_*' \text{ a.c. on } \mathring{\mathbb{R}}, \ \psi_*, \hat{H}^*\psi_* \in L^2(\mathbb{R})\right\}, \\ \hat{H}^*\psi_*(x) = \check{\mathcal{H}}\psi_*(x), \ x \neq 0; \ \ \hat{H}^*\psi_*(0) = a, \ \forall \psi_* \in D^*_{\check{H}}\left(\mathring{\mathbb{R}}\right), \end{cases}$$

where a is an arbitrary constant.

Using the Lemma 2.14, one can easily verify that functions $\psi_* \in D^*_{\check{H}}(\mathbb{R})$ have the following asymptotic behavior at infinity: $\psi_*(x), \psi_*'(x) \overset{|x|\to\infty}{\longrightarrow} 0$. To find the behavior of functions ψ_* at the origin, we consider the condition $\hat{H}^*\psi_* = \eta \in L^2(\mathbb{R})$ as an equation for ψ_*. The general solution of such an equation reads

$$\psi_*(x) = c_1 + c_2 x + \int_0^x (y - x)\eta(y)\mathrm{d}y,$$

which implies

$$|\psi_*(\pm 0)| < \infty; \ \ |\psi_*'(\pm 0)| < \infty, \ \forall \psi_* \in D^*_{\check{H}}\left(\mathring{\mathbb{R}}\right),$$

$$\psi_*(\pm 0) = \lim_{x\to\pm 0} \psi_*(x), \ \ \psi_*'(\pm 0) = \lim_{x\to\pm 0} \psi_*'(x).$$

In addition, the following relation holds:

$$\left(\psi_*, \hat{H}\psi\right) = \left(\hat{H}^*\psi_*, \psi\right), \ \forall\psi \in \mathcal{D}\left(\mathring{\mathbb{R}}\right), \ \forall\psi_* \in D^*_{\check{H}}(\mathbb{R}). \tag{7.75}$$

Let us now demonstrate that $\hat{H}^+$ and $\hat{H}^*$ coincide. We first note that relation (7.75) implies the inclusion $\hat{H}^+ \supseteq \hat{H}^*$. Below, we show that the inverse inclusion $\hat{H}^+ \subseteq \hat{H}^*$ holds as well.

Let $\xi \in D_{H^+}$, i.e.,

$$\xi \in L^2(\mathbb{R}), \ \hat{H}^+\xi = \eta \in L^2(\mathbb{R}), \ \left(\xi, \hat{H}\psi\right) = (\eta, \psi), \ \forall\psi \in \mathcal{D}\left(\mathring{\mathbb{R}}\right), \tag{7.76}$$

and let ζ be an ordinary solution of the equation $\hat{H}\zeta = \eta \in L^2(\mathbb{R})$ (we recall that ζ, ζ' are a.c. on $\mathring{\mathbb{R}}$). Then it follows from (7.76) that

$$\int_0^\infty \overline{[\xi(x) - \zeta(x)]}\check{\mathcal{H}}\psi(x) = 0, \ \forall\psi \in \mathcal{D}(\mathbb{R}_+),$$
$$\int_{-\infty}^0 \overline{[\xi(x) - \zeta(x)]}\check{\mathcal{H}}\psi(x) = 0, \ \forall\psi \in \mathcal{D}(\mathbb{R}_-). \tag{7.77}$$

According to Lemma 4.3, (7.77) implies that, excluding the point $x = 0$, the function $\xi(x)$ can differ from $\zeta(x)$ by a function $u(x)$ that is a solution of the equation $\check{\mathcal{H}}u(x) = 0$. Such a solution reads

$$u(x) = \begin{cases} c_{1+} + c_{2+}x, \ x > 0, \\ c_{1-} + c_{2-}x, \ x < 0, \end{cases}$$

where $c_{1\pm}$ and $c_{2\pm}$ are arbitrary constants.

Therefore, the functions $\xi(x) \in D_{H^+}$ have the properties: $\xi(x) \in L^2(\mathbb{R})$, ξ, ξ' are a.c. on $\mathring{\mathbb{R}}$, and the operator $\hat{H}^*$ is defined on the domain D_{H^+}, because $\hat{H}^*\xi = \check{\mathcal{H}}\xi = \eta = \hat{H}^+\xi \in L^2(\mathbb{R})$, which means that

$$\left.\begin{array}{l} \xi \in D_{H^+} \Longrightarrow \xi \in D_{H^*} \\ \hat{H}^*\xi = \hat{H}^+\xi, \end{array}\right\} \Longrightarrow \hat{H}^+ \subseteq \hat{H}^*,$$

which completes the proof of the equality $\hat{H}^+ = \hat{H}^*$.

We stress that the operator $\hat{H}^+$ acts on its domain as $\check{\mathcal{H}}$ for any $x \neq 0$, and one can define $\hat{H}^+\xi(0) = a$ in an arbitrary way. Recall that two functions $\psi_1, \psi_2 \in L^2(\mathbb{R})$ are considered equivalent if they differ on a set of zero Lebesgue measure; see Sect. 2.1.

Having $\hat{H}^+$ in hand, we calculate the asymmetry form

$$\begin{aligned} \Delta_{H^+}(\psi_*) &= \overline{\psi_*(+0)}\psi_*'(+0) - \overline{\psi_*'(+0)}\psi_*(+0) \\ &\quad - \overline{\psi_*(-0)}\psi_*'(-0) + \overline{\psi_*'(-0)}\psi_*(-0) = \frac{i}{2\kappa_0}(\mathbf{c}^+\mathbf{c} - \mathbf{d}^+\mathbf{d}), \end{aligned} \tag{7.78}$$

where κ_0 is a fixed parameter of dimension of inverse length, and

$$\mathbf{c} = \begin{pmatrix} \kappa_0\psi(+0) - i\psi'(+0) \\ \kappa_0\psi(-0) + i\psi'(-0) \end{pmatrix}, \ \mathbf{d} = \begin{pmatrix} \kappa_0\psi(+0) + i\psi'(+0) \\ \kappa_0\psi(-0) - i\psi'(-0) \end{pmatrix}.$$

The structure (7.78) of an asymmetry form implies that the deficiency indices of $\hat{H}$ are $m_\pm = 2$. The condition $\Delta_{H^+}(\psi_*) = 0$ reduces the space $D^*_{\check{H}}(\mathbb{R})$, imposing restrictions

$$\mathbf{c}^+\mathbf{c} - \mathbf{d}^+\mathbf{d} = 0 \Longrightarrow \mathbf{d} = U\mathbf{c}, U \in U(2), \tag{7.79}$$

on possible functions from $D^*_{\check{H}}(\mathbb{R})$.

Thus, there exists a $U(2)$ family of s.a. extensions $\hat{H}_U$ of the initial symmetric operator $\hat{H}$, acting on their domains D_{H_U},

$$\hat{H}_U : \begin{cases} D_{H_U} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}), \ \mathbf{d} = U\mathbf{c}, \ U \in U(2)\right\}, \\ \hat{H}_U\psi(x) = \check{\mathcal{H}}\psi(x), \ x \neq 0; \ \hat{H}_U\psi(0) = a, \ \forall\psi \in D_{H_U}. \end{cases}$$

7.3.2 Parity Considerations

Let $\hat{P}$ be the parity operator that acts on functions $\psi(x)$ from $L^2(\mathbb{R})$ as

$$\hat{P}\psi(x) = \psi(-x). \tag{7.80}$$

The Hilbert space $L^2(\mathbb{R})$ can be decomposed into the direct orthogonal sum of a subspace $L^2_s(\mathbb{R})$ of symmetric functions ψ_s, $\hat{P}\psi_s = \psi_s$, and a subspace $L^2_a(\mathbb{R})$ of antisymmetric functions ψ_a, $\hat{P}\psi_a = -\psi_a$, so that $L^2(\mathbb{R}) = L^2_s(\mathbb{R}) \oplus L^2_a(\mathbb{R})$. One can easily see that $[\hat{P}, \hat{H}] = [\hat{P}, \hat{H}^+] = 0$. Indeed, acting rules of the operators commute with $\hat{P}$, and their domains are invariant with respect to (7.80). This means that the operators $\hat{H}$ and $\hat{H}^+$ can be represented in the form of a direct sum of their parts, acting in the corresponding subdomains of symmetric and antisymmetric functions:

$$\begin{aligned}
&\hat{H} = \hat{H}_s \oplus \hat{H}_a, \ \hat{H}\psi = \hat{H}_s\psi_s + \hat{H}_a\psi_a, \ \psi = \psi_s + \psi_a, \\
&\psi \in \mathcal{D}\left(\mathring{\mathbb{R}}\right) = \mathcal{D}_s\left(\mathring{\mathbb{R}}\right) \oplus \mathcal{D}_a\left(\mathring{\mathbb{R}}\right), \ \psi_{s,a} \in \mathcal{D}_{s,a}\left(\mathring{\mathbb{R}}\right), \\
&\hat{H}^+ = \hat{H}^+_s \oplus \hat{H}^+_a, \ \hat{H}^+\psi_* = \hat{H}^+_s\psi_{*s} + \hat{H}^+_a\psi_{*a}, \ \psi_* = \psi_{*s} + \psi_{*a}, \\
&\psi_* \in D^*_{\check{H}}(\mathbb{R}) = D^*_{\check{H}}(\mathbb{R})_s \oplus D^*_{\check{H}}(\mathbb{R})_a.
\end{aligned}$$

Owing to the fact that the operator $\hat{P}$ is bounded, $\|\hat{P}\| = 1$, and $\hat{P}^2 = 1$, the assertion that $\hat{P}$ commutes with $\hat{H}_U$ means that

$$[\hat{P}, \hat{H}_U] = 0 \Longrightarrow \hat{H}_U = \hat{H}_{s,U} \oplus \hat{H}_{a,U}, \tag{7.81}$$

where operators $\hat{H}_{s,a,U}$ are s.a. extensions of the operators $\hat{H}_{s,a}$. In turn, if $\hat{H}_{s,a,U}$ are s.a. extensions of $\hat{H}_{s,a}$ in $L^2_{s,a}(\mathbb{R})$, then the operator $\hat{H}_U = \hat{H}_{s,U} \oplus \hat{H}_{a,U}$ is an s.a. extension of $\hat{H}$ in $L^2(\mathbb{R})$ that commutes with $\hat{P}$. Thus, it is enough to describe all s.a. extensions of operators $\hat{H}_{s,a}$ in the subspaces $L^2_{s,a}(\mathbb{R})$ to find all s.a. extensions $\hat{H}_U$ of the operator $\hat{H}$ commuting with $\hat{P}$. This will be done in the next section. Here, finishing the present section, we represent the general form of a matrix U_P conserving parity (commuting with $\hat{P}$).

We start with the remark that the commutativity U with $\hat{P}$ implies that functions $\psi_{s,a} \in L^2_{s,a}(\mathbb{R})$ obey (7.78). On the other hand, functions $\psi_{s,a}$ have the properties

$$\psi_{s,a}(-0) = \pm\psi_{s,a}(+0), \;\; \psi'_{s,a}(-0) = \mp\psi'_{s,a}(+0), \tag{7.82}$$

so that the corresponding doublets $\mathbf{d}_{s,a}$ and $\mathbf{c}_{s,a}$ from (7.78) are

$$\begin{aligned}
\mathbf{d}_{s,a} &= \sqrt{2}[\kappa_0\psi_{s,a}(+0) + i\psi'_{s,a}(+0)]\mathbf{n}_{s,a}, \\
\mathbf{c}_{s,a} &= \sqrt{2}[\kappa_0\psi_{s,a}(+0) - i\psi'_{s,a}(+0)]\mathbf{n}_{s,a}, \\
\mathbf{n}_s &= \left(1/\sqrt{2}\big/1/\sqrt{2}\right), \;\; \mathbf{n}_a = \left(1/\sqrt{2}\big/-1/\sqrt{2}\right).
\end{aligned}$$

It follows from (7.79) that doublets $\mathbf{n}_{s,a}$ are eigenvectors of the matrix U_P defined above,

$$\begin{aligned}
U_P\mathbf{n}_{s,a} &= \lambda_{s,a}\mathbf{n}_{s,a}, \;\; \lambda_{s,a} = \frac{\kappa_0\psi_{s,a}(+0) + i\psi'_{s,a}(+0)}{\kappa_0\psi_{s,a}(+0) - i\psi'_{s,a}(+0)}, \\
\lambda_{s,a} &= \mathrm{e}^{i\varphi_{s,a}}, \;\; \varphi_{s,a} \in \mathbb{S}(-\pi, \pi)\,.
\end{aligned} \tag{7.83}$$

The general form of the U_P satisfying condition (7.83) is

$$U_P = \lambda_s\mathbf{n}_s \otimes \mathbf{n}_s + \lambda_s\mathbf{n}_s \otimes \mathbf{n}_s. \tag{7.84}$$

The inverse statement is true as well. Namely, if a matrix U has the form (7.84), then the subspaces $L^2_{s,a}(\mathbb{R})$ reduce the corresponding s.a. Hamiltonian $\hat{H}_U$, i.e., (7.81) takes place.

In terms of a.b. conditions, such a form of the matrix U_P implies

$$\psi'_{s,a}(+0)\cos\zeta_{s,a} = \kappa_0\psi_{s,a}(+0)\sin\zeta_{s,a}, \;\; \zeta_{s,a} \in \mathbb{S}(-\pi/2, \pi/2)\,, \tag{7.85}$$

where $\zeta_{s,a} = \varphi_{s,a}/2$. The inverse statement is true as well. Namely, if a matrix U_P implies a.b. boundary conditions of the form (7.85), then it has the form (7.84) with $\varphi_{s,a} = 2\zeta_{s,a}$.

7.3.2.1 Self-adjoint Extensions of $\hat{H}_s$

Functions $\psi, \chi \in L_s^2(\mathbb{R})$ satisfy the relations (7.82) which implies

$$(\chi, \psi) = 2(\chi, \psi)_+, \ \Delta_{H^+}(\psi) = 2(\psi, \psi)_+,$$

where

$$(\chi, \psi)_+ = \int_0^\infty \overline{\chi(x)}\psi(x)\,\mathrm{d}x, \tag{7.86}$$

and $\Delta_{H^+}(\psi)_+$ is the asymmetry form with respect to the scalar product (7.86).

Let us consider the isometry T: $\psi \in \mathbb{R} \xrightarrow{T} \sqrt{2}\psi \in \mathbb{R}_+$. Then

$$D_{H_s} \xrightarrow{T} D_{\mathcal{H}} = \mathcal{D}(\mathbb{R}_+), \ \ D_{H_s^+} \xrightarrow{T} D_{\mathcal{H}^+} = D^*_{\check{H}}(\mathbb{R}_+). \tag{7.87}$$

It follows from (7.87) that there is a one-to-one correspondence (the isometry T) between s.a. extensions $\hat{H}_{s,U}$ and s.a. Hamiltonians $\widehat{\mathcal{H}}_U$ of the free particle on the semiaxis. The latter extensions were described in detail in Sect. 6.2. Using these results we obtain that there is a family of s.a. Hamiltonians $\hat{H}_{s,\zeta}$, $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$, defined on the domain $D_{H_{s,\zeta}}$,

$$D_{H_{s,\zeta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R})_s, \ \psi'(+0)\cos\zeta = \kappa_0\psi(+0)\sin\zeta\right\},$$

where they act as $\check{\mathcal{H}}$.

For $\zeta \geq 0$ or $\zeta = -\pi/2$, the spectrum of $\hat{H}_{s,\zeta}$ is continuous and simple, spec $\hat{H}_{s,\zeta} = \mathbb{R}_+$. The generalized eigenfunctions $U_E(x)$, $E \geq 0$,

$$U_E(x) = \sqrt{\frac{2m}{\pi\left[\cos^2\zeta + \left(\kappa_0^2/E\right)\sin^2\zeta\right]}}\left[\cos\left(\sqrt{E}x\right)\cos\zeta + \kappa_0\frac{\sin\left(\sqrt{E}|x|\right)}{\sqrt{E}}\sin\zeta\right],$$

form a complete orthonormalized system in $L_s^2(\mathbb{R})$.

For $-\pi/2 < \zeta < 0$, the spectrum of $\hat{H}_{s,\zeta}$ is simple and, in addition to the previous positive continuous part, contains a negative level,

$$\text{spec } \hat{H}_{s,\zeta} = \mathbb{R}_+ \cup \left\{-\frac{(\kappa_0\tan\zeta)^2}{2m}\right\}.$$

The generalized eigenfunctions $U_E(x)$, $E \geq 0$, and an eigenfunction $U(x)$,

$$U(x) = \sqrt{\kappa_0 \tan|\zeta|}\mathrm{e}^{-\kappa_0|x \tan\zeta|},$$

form a complete and orthonormalized system in $L_s^2(\mathbb{R})$.

7.3.2.2 Self-adjoint Extensions of $\hat{H}_a$

Using similar arguments, one can see that there is a one-to-one correspondence (the isometry T) between s.a. extensions $\hat{H}_{a,U}$ and s.a. Hamiltonians $\widehat{\mathcal{H}}_U$ of the free particle on the semiaxis. Therefore, there is a family of s.a. Hamiltonians $\hat{H}_{a,\zeta}$, $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$, defined on the domain $D_{H_{a,\zeta}}$,

$$D_{H_{a,\zeta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R})_a\,,\ \psi'(+0)\cos\zeta = \kappa_{\not{\,}}\psi(+0)\sin\zeta\right\},$$

where they act as $\check{\mathcal{H}}$.

For $\zeta \geq 0$, the simple spectrum of $\hat{H}_{a,\zeta}$ is given by spec $\hat{H}_{a,\zeta} = \mathbb{R}_+$.

The generalized eigenfunctions $U_E(x)$, $E \geq 0$,

$$U_E(x) = \sqrt{\frac{2m}{\pi\left[\cos^2\zeta + \left(\kappa_0^2/E\right)\sin^2\zeta\right]}}\left[\frac{x}{|x|}\cos\left(\sqrt{E}x\right)\cos\zeta + \frac{\kappa_0\sin\left(\sqrt{E}x\right)}{\sqrt{E}}\sin\zeta\right],$$

form a complete orthonormalized system in $L_a^2(\mathbb{R})$.

For $-\pi/2 < \zeta < 0$, the spectrum of $\hat{H}_{a,\zeta}$ is simple and, in addition to the previous positive continuous part, contains a negative level,

$$\mathrm{spec}\,\hat{H}_{a,\zeta} = \mathbb{R}_+ \cup \left\{-\frac{(\kappa_0\tan\zeta)^2}{2m}\right\}.$$

The generalized eigenfunctions $U_E(x)$, $E \geq 0$, and an eigenfunction $U(x)$,

$$U(x) = (\mathrm{sgn}\,x)\sqrt{\kappa_0\tan|\zeta|}\mathrm{e}^{-\kappa_0|x\tan\zeta|},$$

form a complete orthonormalized system in $L_a^2(\mathbb{R})$.

For s.a. Hamiltonians $\hat{H}_{U_P}$ that commute with $\hat{P}$, we have

$$\hat{H}_{U_P} = \hat{H}_{s,\zeta_s} \oplus \hat{H}_{a,\zeta_a},\ \zeta_s, \zeta_a \in \mathbb{S}(-\pi/2, \pi/2),$$
$$\mathrm{spec}\,\hat{H}_{U_P} = \mathrm{spec}\,\hat{H}_{s,\zeta_s} \cup \mathrm{spec}\,\hat{H}_{a,\zeta_a},$$

where the eigenfunctions of the s.a. Hamiltonians $\hat{H}_{U_P}$ and the corresponding inversion formulas are the respective unions of the eigenfunctions of $\hat{H}_{s,\zeta_s}$ and $\hat{H}_{a,\zeta_a}$ and the corresponding inversion formulas (for $\hat{H}_{s,\zeta_s}$ and $\hat{H}_{a,\zeta_a}$).

7.3.3 Self-adjoint Schrödinger Operators with δ-Potential

Below, we apply the above results to the old problem of particle motion in a δ-potential field; see [3,26,94]. We need to find a matrix U such that the corresponding s.a. Hamiltonian $\hat{H}_U$ can be physically interpreted as a Hamiltonian describing the motion of a particle in a δ-potential field.

Let us now recall the well-known consideration that allows one to reformulate the QM problem with poorly defined Schrödinger operator (in fact, for the Schrödinger differential operation with δ-potential) in terms of some boundary conditions. For example, let us consider the stationary Schrödinger equation of the form

$$\left[-d_x^2 + g\delta(x)\right]\psi(x) = E\psi(x), \tag{7.88}$$

where g is a coupling constant. We suppose that $\psi(x)$ is continuous at the origin (otherwise, the product $\delta(x)\psi(x)$ is not well defined). Integrating the left and the right sides of (7.88) over x in the limits $-\varepsilon$ and ε and considering the limit $\varepsilon \to 0$, we find that solutions of (7.88) must obey the boundary conditions

$$\psi(0) = \frac{1}{g}[\psi'(+0) - \psi'(-0)]. \tag{7.89}$$

Considering a nonstationary or inhomogeneous Schrödinger equation implies the same result.

One can see that the boundary condition (7.89), together with continuity of the wave function at the origin, coincides with some s.a. boundary conditions for s.a. extensions of the initial symmetric operator $\hat{H}$.

Indeed, being rewritten in terms of symmetric and antisymmetric components, (7.89) takes the form

$$\psi_a(+0) = 0,\ \psi_s(+0) = \frac{1}{2g}\psi_s'(+0). \tag{7.90}$$

The boundary conditions (7.90) correspond to doublets $\mathbf{d}$ and $\mathbf{c}$ having the form

$$\mathbf{d} = \sqrt{2}(1 + i/2g)\psi_s(+0)\mathbf{n}_s + i\sqrt{2}\psi_s'(+0)\mathbf{n}_a,$$
$$\mathbf{c} = \sqrt{2}(1 - i/2g)\psi_s(+0)\mathbf{n}_s - i\sqrt{2}\psi_s'(+0)\mathbf{n}_a,$$

so that the corresponding matrix U reads

$$U = U_P = (2g - i)^{-1}(2g + i)\mathbf{n}_s \otimes \mathbf{n}_s - \mathbf{n}_a \otimes \mathbf{n}_a.$$

It coincides with the matrix (7.84) for

$$\varphi_s = 2 \arcsin \frac{\operatorname{sgn} g}{\sqrt{1 + 4g^2}}, \quad \varphi_a = \pm\pi.$$

Such a matrix U specifies s.a. operators of the form

$$\hat{H}_{U_P} = \hat{H}_{s,\zeta_s} \oplus \hat{H}_{a,\zeta_a}, \quad \zeta_s = \arcsin \frac{\operatorname{sgn} g}{\sqrt{1 + 4g^2}}, \quad \zeta_a = \pm\pi/2, \tag{7.91}$$

conserving the parity (commuting with $\hat{P}$). Thus, s.a. operators (7.91) can be identified with s.a. Schrödinger operators that describe one-dimensional particle motion in the δ-potential. The spectrum and inversion formulas for such operators can be extracted from the above considerations depending on concrete values of parameters g and κ_0.

Remark 7.3. Regarding the potential $V^\circ(x) = \delta'(x)$, one can meet in the literature (see, e.g., [3]) a supposition that the domain of an s.a. Schrödinger operator with the potential $V^\circ(x) = \delta'(x)$ is defined by s.a. boundary conditions

$$\kappa_0\psi(+0) - \kappa_0\psi(-0) = g\psi'(+0), \quad \psi'(+0) = \psi'(-0). \tag{7.92}$$

Indeed, s.a. boundary conditions (7.92) correspond to an s.a. Schrödinger operator with a potential $V^\circ(x)$ localized at the origin. One can verify that they correspond to the following matrix U:

$$U = U_P = \mathbf{n}_s \otimes \mathbf{n}_s + (g - 2i)^{-1}(g + 2i)\mathbf{n}_a \otimes \mathbf{n}_a,$$

which defines a an s.a. Schrödinger operator that conserves the parity (commutes with P). For this reason, such an operator cannot correspond to the potential $V^\circ(x) = \delta'(x)$; the latter potential is not invariant under the transformation $x \to -x$.

Chapter 8
Schrödinger Operators with Exactly Solvable Potentials

It is known that an infinite number of potentials $V(x)$ admit exact solutions of the one-dimensional (stationary) Schrödinger equation (7.2). Below, we are going to study some of them that are of prime importance. We consider all the potentials of the form

$$V(x) = \sum_i g_i v_i(x),$$

where g_i are arbitrary constants, for which the one-dimensional Schrödinger equation has a general solution in terms of elementary or special functions for all values of parameters g_i. In particular, potentials of such a form usually arise as a result of separating variables in the course of solving the nonrelativistic and relativistic wave equations in $3+1$ or $2+1$ dimensions. Potentials resulting from these manipulations depend on the separation constants g_i (being integrals of motion).

We are also interested in having not just one, or several, solutions of (7.2) for a given potential and some values of the energy, but in a sense (see Chap. 5), a complete set of solutions. Potentials that admit a solution of the one-dimensional Schrödinger equation in this sense will be called *exactly solvable potentials* (*ESP*).

There exist eleven types of potentials that are candidates for ESP; see, e.g., [13]. Below, we study the one-dimensional Schrödinger equation with such potentials, constructing the corresponding s.a. Schrödinger Hamiltonians and solving the corresponding spectral problems. In each section below, we start with a specification of the ESP $V(x)$ in the Schrödinger differential operation $\check{H} = -d_x^2 + V(x)$, and with the corresponding one-dimensional Schrödinger equation.

8.1 ESP I

In this case,

$$V(x) = cx, \quad x \in \mathbb{R},$$

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and the corresponding Schrödinger equation is

$$\psi'' - cx\psi + W\psi = 0. \tag{8.1}$$

It is sufficient to consider only the case $c > 0$. The case with a negative c can be reduced to the previous one by the transformation $x \to -x$ in (8.1).

The initial symmetric Schrödinger operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}(\mathbb{R})$. Its adjoint $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R})$, where it acts as $\check{H}$, i.e., $D_{H^+} = D^*_{\check{H}}(\mathbb{R})$. As follows from results of Sect. 7.1, $[\psi_*, \psi_*](\pm\infty) = 0$, $\forall \psi_* \in D^*_{\check{H}}(\mathbb{R})$, because $V(x) > -x^{-2}$ as $x \to \infty$. Thus, we have $\Delta_{H^+}(\psi_*) = 0$. Therefore the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

Let us introduce new variables y and υ, and a new function $\phi(x)$, instead of x and $\psi(x)$ in (8.1),

$$y = c^{1/3}(x - W/c), \ \upsilon = \frac{2}{3}y^{3/2}, \ \psi(x) = \sqrt{y}\phi(\upsilon). \tag{8.2}$$

Then $\phi(y)$ obeys the Bessel equation

$$d_\upsilon^2\phi + \upsilon^{-1}d_\upsilon\phi - \left[1 + (3\upsilon)^{-2}\right]\phi = 0\,.$$

Solutions of (8.1) can be obtained from solutions of the Bessel equation by the transformation (8.2).

As a fundamental set of solutions of (8.1), we chose $u_i(x; W)$, $i = 1, 2$,

$$\begin{aligned} u_1(x; W) &= \sqrt{y}K_{1/3}(\upsilon) = \pi\sqrt{y/3}[I_{-1/3}(\upsilon) - I_{1/3}(\upsilon)] \\ &= \pi\sqrt{\widetilde{y}/3}[J_{1/3}(\widetilde{\upsilon}) + J_{-1/3}(\widetilde{\upsilon})], \ \widetilde{y} = c^{1/3}(W/c - x), \ \widetilde{\upsilon} = \frac{2}{3}\widetilde{y}^{3/2}, \\ u_2(x; W) &= \sqrt{y}\left[K_{1/3}(\upsilon) + \pi e^{-i\pi/6}I_{1/3}(\upsilon)\right] = \frac{i\pi}{2}\sqrt{\widetilde{y}}H^{(1)}_{1/3}(\widetilde{\upsilon}), \end{aligned} \tag{8.3}$$

where I_ν and K_ν are Bessel functions of an imaginary argument [1, 20, 81]. In (8.3) we have used the following relations:

$$\sqrt{y}I_{1/3}(\upsilon) = \sqrt[3]{c/3}(x - W/c)\sum_{k=0}^{\infty}\frac{c^k(x - W/c)^{3k}}{3^{2k}\Gamma(4/3 + k)k!} = -\sqrt{\widetilde{y}}J_{1/3}(\widetilde{\upsilon}),$$

$$\sqrt{y}I_{-1/3}(\upsilon) = \sum_{k=0}^{\infty}\frac{c^k(x - W/c)^{3k}}{3^{2k}\Gamma(2/3 + k)k!} = \sqrt{\widetilde{y}}J_{-1/3}(\widetilde{\upsilon}).$$

The representation of the solutions in terms of the variables $\widetilde{y}$ and $\widetilde{\upsilon}$ is useful for finding asymptotics as $x \to -\infty$. We note that $u_1(x; W)$ is a real entire function of W and $u_2(x; W)$ is an entire function of W.

Denoting $W/c = a + ib$, and taking into account that[1]

$$
\begin{aligned}
&y = c^{1/3} x \tilde{O}\left(x^{-1}\right),\ x \to \infty,\\
&\upsilon = c^{1/2}\left(2x^{3/2}/3 - ax^{1/2} - ibx^{1/2}\right) + O\left(x^{-1/2}\right),\ x \to \infty,\\
&\widetilde{y} = c^{1/3}|x|\tilde{O}(|x|^{-1}),\ x \to -\infty,\\
&\widetilde{\upsilon} = 2c^{1/2}\left(|x|^{3/2}/3 + a|x|^{1/2}/2\right) + bc^{1/2}|x|^{1/2} + O\left(|x|^{-1/2}\right),\ x \to -\infty,
\end{aligned}
$$

we obtain the asymptotic of $u_i\ (x; W)$ as $|x| \to \infty$:

1. $W \in \mathbb{C},\ x \to \infty$:

$$
\begin{aligned}
u_1 &= \sqrt{3\pi/4}\left(c^{1/3}x\right)^{-1/4} \mathrm{e}^{-\frac{2c^{1/2}}{3}\left(x^{3/2} - \frac{3}{2}ax^{1/2}\right) - ibc^{1/2}x^{1/2}} + O(x^{-3/4}) \to 0,\\
u_2 &= \sqrt{3\pi/4}\left(c^{1/3}x\right)^{-1/4} \mathrm{e}^{i\pi/6 + \frac{2c^{1/2}}{3}\left(x^{3/2} - \frac{3a}{2}x^{1/2}\right) - ibc^{1/2}x^{1/2}} + O(x^{-3/4}) \to \infty.
\end{aligned}
$$

2. $\operatorname{Im} W/c = b > 0,\ x \to -\infty$:

$$
\begin{aligned}
u_1 &= \sqrt{3\pi/4}\left(c^{1/3}|x|\right)^{-1/4} \mathrm{e}^{-i\left[\frac{2c^{1/2}}{3}\left(|x|^{3/2} + \frac{3a}{2}|x|^{1/2}\right) - \frac{\pi}{4}\right] + bc^{1/2}|x|^{1/2}}\\
&\quad + O\left(|x|^{-3/4}\right) \to \infty,\\
u_2 &= i\sqrt{3\pi/4}\left(c^{1/3}|x|\right)^{-1/4} \mathrm{e}^{i\left[\frac{2c^{1/2}}{3}\left(|x|^{3/2} + \frac{3a}{2}|x|^{1/2}\right) - \frac{5\pi}{12}\right] - bc^{1/2}|x|^{1/2}}\\
&\quad + O\left(|x|^{-3/4}\right) \to 0.
\end{aligned}
$$

3. $\operatorname{Im} W/c = b = 0,\ a = E/c,\ x \to -\infty$:

$$
\begin{aligned}
u_1 &= \sqrt{3\pi}\left(c^{1/3}|x|\right)^{-1/4} \cos\left(X - \pi/4\right) + O\left(|x|^{-3/4}\right),\\
u_2 &= -\sqrt{3\pi/4}\left(c^{1/3}|x|\right)^{-1/4} \mathrm{e}^{i(X + \pi/12)} + O\left(|x|^{-3/4}\right),\\
X &= 2c^{1/2}\left(|x|^{3/2}/3 + E\,|x|^{1/2}/2c\right).
\end{aligned}
$$

Since $\mathrm{Wr}\,(u_1, u_2)$ does not depend on x, one can calculate it using the above asymptotics. Thus, we obtain

$$
\mathrm{Wr}\,(u_1, u_2) = \frac{3\pi}{2}c^{1/3}\mathrm{e}^{-i\pi/6} \equiv w \neq 0,
$$

[1] We recall that $\tilde{O}\,(x) = 1 + O\,(x)$.

which means that u_1 and u_2 are linearly independent and form a fundamental set of solutions of (8.1). One can see that any linear combination of the fundamental set is not square-integrable for any $W \in \mathbb{C}$. This means that the deficiency indices of $\hat{H}$ are zero. The fact that $u_{1,2}(x; E) \notin L^2(\mathbb{R})$ implies the absence of bound states for the linear potential under consideration. However, we note that $u_1 \in L^2(-\infty, x_0)$ and $u_2 \in L^2(x_0, \infty)$ for any finite x_0. This fact will be used in constructing a Green's function of the s.a. $\hat{H}_1$.

One can see that u_1 decreases exponentially for big x, which is matched with the physical expectation about the behavior of the wave function in classically forbidden areas.

The general solution of the inhomogeneous equation

$$\left(\check{H} - W\right) \xi(x) = \eta(x) \in L^2(\mathbb{R}), \;\; \operatorname{Im} W \neq 0,$$

has the form

$$\xi(x) = c_1 u_1(x; W) + c_2 u_2(x; W) + w^{-1}(W) \\ \times \left[u_1(x; W) \int_{-\infty}^{x} u_2(y; W)\eta(y)\mathrm{d}y + u_2(x; W) \int_{x}^{\infty} u_1(y; W)\eta(y)\mathrm{d}y \right],$$

where $c_{1,2}$ are arbitrary constants. With the help of the Cauchy–Schwarz inequality, we can verify that both terms in square brackets are bounded as $|x| \to \infty$, which implies that $c_1 = c_2 = 0$ must hold if $\xi \in L^2(\mathbb{R})$. Then following Sect. 5.3.4, we find the Green's function of the operator $\hat{H}_1$,

$$G(x, y; W) = w^{-1} u_1(x; W) u_1(y; W) \\ + \frac{2}{3c^{1/3}} \begin{cases} \tilde{G}^{(+)}(x, y; W), & x > y, \\ \tilde{G}^{(-)}(x, y; W), & x < y, \end{cases} \tag{8.4}$$

where

$$G^{(+)}(x, y; W) = u_1(x; W)u_2(y; W), \;\; G^{(-)}(x, y; W) = u_2(x; W)u_1(y; W),$$
$$\tilde{G}^{(+)}(x, y; W) = u_1(x; W)u_3(y; W), \;\; \tilde{G}^{(-)}(x, y; W) = u_3(x; W)u_1(y; W),$$
$$u_3(x; W) = y^{1/2} I_{1/3}(\upsilon).$$

We stress that $u_3(x; W)$ is a real entire function in W, and therefore, the functions $\tilde{G}^{(\pm)}(x, y; W)$ are real for $\operatorname{Im} W = 0$.

Let us consider the guiding functional

$$\Phi(\xi; W) = \int_{\mathbb{R}} u_1(x; z)\xi(x)\mathrm{d}x, \;\; \xi \in \mathbb{D} = \mathcal{D}_l(\mathbb{R}) \cap D^*_{\check{H}}(\mathbb{R}).$$

Properties (i) and (iii) (see Sect. 5.3) for $\Phi(\xi; W)$ to be simple are obviously fulfilled. We need only check Property (ii). Let there exist $\xi_0(x) \in \mathbb{D}$ and $E_0 \in \mathbb{R}$ such that

$$\Phi(\xi_0; E_0) = \int_{-\infty}^{\infty} \mathrm{d}x\, u_1(x; E_0)\, \xi_0(x) = \int_a^{\infty} \mathrm{d}x\, u_1(x; E_0)\, \xi_0(x) = 0, \quad (8.5)$$

where $\operatorname{supp} \xi_0 \in [a, \infty)$. Consider a solution

$$\psi(x) = \frac{1}{w}\left[\int_a^x G^{(+)}(x, y; E_0)\, \xi_0(y)\, \mathrm{d}y + \int_x^{\infty} G^{(-)}(x, y; E_0)\, \xi_0(y)\, \mathrm{d}y\right] \quad (8.6)$$

of the equation $\left(\check{H} - E_0\right)\psi = \xi_0$. Since $\xi_0(x)$ is compact on $-\infty$, the function $\psi(x)$ is well defined. Since $\xi_0(x)$ is compact on $-\infty$ and Property (8.5) holds, the function $\psi(x)$ is compact on $-\infty$. One can see that both summands in square brackets of (8.6) behave as $x^{-3/4}$ as $x \to \infty$, which implies that $\psi, \check{H}\psi = \xi_0 + E_0\psi \in L^2(\mathbb{R})$, i.e., $\psi \in \mathbb{D}$. Thus, $\Phi(\xi; W)$ is a simple guiding functional, and the spectrum of the s.a. Hamiltonian $\hat{H}_1$ is simple.

With the help of (5.21), (5.22), and the Green's function (8.4), we obtain the derivative of the spectral function:

$$\sigma'(E) = \pi^{-1} \operatorname{Im} w^{-1} = \pi^{-2} c^{-1/3}/3 > 0.$$

Thus, the simple spectrum of $\hat{H}_1$ reads $\operatorname{spec} \hat{H}_1 = \mathbb{R}$.

The generalized eigenfunctions $U_E(r)$ of $\hat{H}_1$,

$$U_E(x) = \frac{1}{c^{1/6}\pi}\sqrt{y/3}\, K_{1/3}\left(2y^{3/2}/3\right), \quad y = c^{1/3}(x - E/c), \; E \in \mathbb{R},$$

form a complete and orthonormalized system in $L^2(\mathbb{R})$. Formally, the latter means that relation (5.24) must hold. Indeed, we can write

$$\begin{aligned}
\int_{-\infty}^{\infty} \mathrm{d}x\, U_E(x)\, U_{E'}(x) &= \int_{-\infty}^{\infty} \mathrm{d}x \left\{U_E(x)\left(\check{H} - E\right) U_E(x)\right. \\
&\quad \left. - \left[\left(\check{H} - E'\right) U_{E'}(x)\right] U_{E'}(x)\right\} = \left[\left(E - E'\right) 3\pi^2\right]^{-1} \\
&\quad \times \left[\sqrt{y}\, y' K_{1/3}(\upsilon)\, K_{2/3}(\upsilon') - y\sqrt{y'} K_{2/3}(\upsilon)\, K_{1/3}(\upsilon')\right]_{x \to -\infty} \\
&= \left[\pi\left(E - E'\right)\right]^{-1} \sin\left[\left(E - E'\right)\left(2\,|cx|^{1/2}/3\right)\right]_{|x| \to \infty} = \delta\left(E - E'\right). \quad (8.7)
\end{aligned}$$

In the course of the calculations, we have omitted terms that vanish as $x \to -\infty$, and have used the well-known relation $\lim_{R\to\infty} E^{-1} \sin(ER) = \pi\delta(E)$. To obtain the second relation (5.24), we note that $U_E(x) = \psi(x - E/c)$. Then it follows from (8.7) that

$$\int_{-\infty}^{\infty} \mathrm{d}x\, U_E(x)\, U_{E'}(x) = \int_{-\infty}^{\infty} \mathrm{d}z \psi(z)\, \psi(z + \Delta/c) = \delta(\Delta)\,,\ \Delta = E - E',$$

and therefore,

$$\int_{-\infty}^{\infty} \mathrm{d}E\, U_E(x)\, U_E(x') = c \int_{-\infty}^{\infty} \mathrm{d}z\, \psi(z)\, \psi\left(z + \tilde{\Delta}/c\right)$$
$$= c\delta\left(\tilde{\Delta}\right) = \delta\left(x - x'\right),\ \ \tilde{\Delta} = c\left(x' - x\right).$$

8.2 ESP II

In this case, we have

$$V(x) = g_1 x^2 + g_2 x,\ \ x \in \mathbb{R}.$$

By a shift of x, one can always reduce the problem to that with $g_2 = 0$. That is why it is sufficient to consider only the case in which $g_1 \equiv g \neq 0$ and $g_2 = 0$. The corresponding Schrödinger equation is

$$\psi'' - gx^2 + W\psi = 0. \tag{8.8}$$

The initial symmetric operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}(\mathbb{R})$ and $D_{H+} = D^*_{\check{H}}(\mathbb{R})$. The potential under consideration obeys the condition $V(x) > -(|g| + 1)x^2$, so that $[\psi_*, \psi_*](\pm\infty) = 0$, as was proved in Sect. 7.1. Thus, for any real g, we have $\Delta_{H+}(\psi_*) = 0$, which implies that the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$. Further analysis will be done separately for the two ranges $g > 0$ and $g < 0$.

8.2.1 Range 1

In this range, we have

$$g = \upsilon^4 > 0,\ \upsilon > 0.$$

Let us introduce a new variable z and a new function ϕ, instead of x and $\psi(x)$ in (8.8),

$$z = (\upsilon x)^2\,,\ \ \psi(x) = \mathrm{e}^{-z/2}\phi(z)\,. \tag{8.9}$$

Then $\phi(y)$ obeys the equation for the confluent hypergeometric function,

$$zd_z^2\phi + (1/2 - z)d_z\phi - \alpha\phi = 0,\ \ \alpha = 1/4 - w,\ w = W/4\upsilon^2\,; \tag{8.10}$$

see [1, 20, 81]. Therefore, solutions of (8.8) can be obtained from solutions of (8.10) by the transformation (8.9). Thus, we obtain a fundamental set $u_{1,2}(x; W)$ of solutions of (8.8),

$$u_{1,2}(x; W) = \sqrt{\pi} e^{-z/2} \left[\frac{\Phi(\alpha, 1/2; z)}{\Gamma(\alpha + 1/2)} \mp \frac{2(\upsilon x)}{\Gamma(\alpha)} \Phi(\alpha + 1/2, 3/2; z) \right], \quad (8.11)$$

where $\Phi(\alpha, \beta; x)$ is the confluent hypergeometric function. Solutions (8.11) are real entire in W for any fixed x, and are independent for $\alpha, \alpha + 1/2 \neq -n$, $n \in \mathbb{Z}_+$, in particular, for $\operatorname{Im} W \neq 0$,

$$\mathrm{Wr}(u_1, u_2) = \frac{4\pi\upsilon}{\Gamma(\alpha)\Gamma(\alpha + 1/2)} \equiv \omega(W).$$

The functions $u_{1,2}$ and their linear combinations are not square-integrable for $\operatorname{Im} W \neq 0$. The latter means that the deficiency indices are zero, which confirms the fact that $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of the initial symmetric operator $\hat{H}$.

For $\alpha, \alpha + 1/2 \neq -n$, $n \in \mathbb{Z}_+$, the solutions $u_{1,2}$ have the following asymptotic behavior as $|x| \to \infty$:

$$\begin{aligned}
u_1 &= e^{-(\upsilon x)^2/2} (\upsilon |x|)^{-1/2+2w} \tilde{O}(x^{-2}) \to 0, \ x \to \infty, \\
u_1 &= \frac{2\pi}{\Gamma(\alpha)\Gamma(\alpha + 1/2)} e^{(\upsilon x)^2/2} (\upsilon |x|)^{-1/2-2w} \tilde{O}(x^{-2}) \to \infty, \ x \to -\infty, \\
u_2 &= \frac{2\pi}{\Gamma(\alpha)\Gamma(\alpha + 1/2)} e^{(\upsilon x)^2/2} (\upsilon |x|)^{-1/2-2w} \tilde{O}(x^{-2}) \to \infty, \ x \to \infty, \\
u_2 &= e^{-(\upsilon x)^2/2} (\upsilon |x|)^{-1/2+2w} \tilde{O}(x^{-2}) \to 0, \ x \to -\infty.
\end{aligned}$$

In finding the asymptotics, we have used the representations

$$\left. \begin{array}{l} u_1(x; W), \ x > 0 \\ u_2(x; W), \ x < 0 \end{array} \right\} = e^{-z/2} \Psi(\alpha, 1/2; z).$$

Following Sect. 5.3.4, we find the Green's function of the operator $\hat{H}_1$,

$$G(x, y; W) = \omega^{-1}(W) \begin{cases} u_1(x; W) u_2(y; W), \ x > y, \\ u_2(x; W) u_1(y; W), \ x < y. \end{cases} \quad (8.12)$$

As in Sect. 7.3.1, one can see that the guiding functional

$$\Phi(\xi; W) = \int_{\mathbb{R}} u_1(x; z) \xi(x) dx, \ \xi \in \mathcal{D}_l(\mathbb{R}) \cap D^*_{\check{H}}(\mathbb{R})$$

is simple, and therefore the spectrum of $\hat{H}_1$ is simple.

With the help of (5.21) and (5.22), the Green's function (8.12), and the fact that $u_{1,2}(c; W)$ are real for real $W = E$, we obtain the derivative of the spectral function:

$$\sigma'(E) = \frac{u_2(c; E)}{4\pi^2 \upsilon u_1(c; E)} \operatorname{Im} \Gamma(\alpha)\Gamma(\alpha + 1/2)|_{W=E+i0},$$

where $c \in \mathbb{R}$ is an arbitrary constant.

The fact that $\operatorname{Im} \Gamma(x) = 0$ for $x \notin \mathbb{Z}_-$ implies that $\sigma'(E) \neq 0$ only for those E for which either $\alpha = -k$ or $\alpha + 1/2 = -k$, $k \in \mathbb{Z}_+$, i.e., for those E that provide poles either for $\Gamma(1/4 - E/(4\upsilon^2))$ or for $\Gamma(3/4 - E/4\upsilon^2)$.

For $\alpha = -k = -n/2$, $n = 2k = 0, 2, 4, \ldots$, and $E_n = 2\upsilon^2(n + 1/2)$, we obtain

$$u_1(x; E_n) = u_2(x; E_n) = (-1/2)^{n/2}(n-1)!!\mathrm{e}^{-z/2}\Phi(-n/2, 1/2; z),$$
$$\frac{u_2(c; E_n)}{u_1(c; E_n)} = 1, \quad \Gamma(\alpha + 1/2) = \frac{(-2)^{n/2}\sqrt{\pi}}{(n-1)!!}.$$

For E in a neighborhood of E_n, one can write (see Lemma 5.17)

$$\operatorname{Im} \Gamma(\alpha)|_{W=E+i0} = \frac{4\pi\upsilon^2(-2)^{n/2}}{n!!}\delta(E - E_n).$$

Then

$$\sigma'(E) = Q_n^2 \delta(E - E_n), \quad Q_n = \sqrt{\frac{2^n \upsilon}{\sqrt{\pi} n!}}.$$

For $\alpha = -k - 1/2 = -n/2$, $n = 2k + 1 = 1, 3, 5, \ldots$, $E_n = 2\upsilon^2(n + 1/2)$, we obtain

$$\begin{aligned}
u_1(x; E_n) &= -u_2(x; E_n) \\
&= (-2)^{1/2-n/2} n!!\mathrm{e}^{-z/2}(\upsilon x)\Phi(-(n-1)/2, 3/2; z), \; z = (\upsilon x)^2, \\
\frac{u_2(c; E_n)}{u_1(c; E_n)} &= -1, \; \Gamma(\alpha) = \frac{(-2)^{k+1}\sqrt{\pi}}{n!!}, \\
\operatorname{Im} \Gamma(\alpha + 1/2)|_{W=E+i0, E\sim E_n} &= \frac{4\upsilon^2\pi(-1)^k}{k!}\delta(E - E_n) \\
&= \frac{4\upsilon^2\pi(-2)^k}{(n-1)!!}\delta(E - E_n),
\end{aligned}$$

and $\sigma'(E) = Q_n^2 \delta(E - E_n)$, so that the simple spectrum of $\hat{H}_1$ reads

$$\operatorname{spec} \hat{H}_1 = \left\{E_n = 2\upsilon^2(n + 1/2), \;\; n \in \mathbb{Z}_+\right\}.$$

It consists of the eigenvalues of $\hat{H}_1$, well known from any textbook.

The functions

$$U_n(x) = Q_n u_1(x; E_n) = \sqrt{\frac{\upsilon}{2^n \sqrt{\pi} n!}} \mathrm{e}^{-\frac{(\upsilon x)^2}{2}} H_n(\upsilon x),$$

which are the standard eigenfunctions of the harmonic oscillator Hamiltonian, form a complete orthonormalized system in $L^2(\mathbb{R})$. Here, we have used relations between the confluent hypergeometric functions and the Hermite polynomials H_n; see, e.g., [81].

8.2.2 Range 2

In this range, we have

$$g = -\upsilon^4 < 0, \ \upsilon > 0.$$

Here we introduce a new variable z and a new function ϕ, instead of x and $\psi(x)$ in (8.8),

$$z = i\,(\upsilon x)^2 = \mathrm{e}^{i\pi/2}\,(\upsilon x)^2\,, \quad \psi(x) = \mathrm{e}^{-z/2}\phi(z)\,. \tag{8.13}$$

Then $\phi(y)$ obeys the equation for the confluent hypergeometric function,

$$z d_z^2 \phi(z) + (1/2 - z) d_z \phi(z) - \alpha\phi(z) = 0, \ \alpha = 1/4 + iw, \ w = W/(4\upsilon^2). \tag{8.14}$$

Therefore, solutions $\psi(x)$ of (8.8) can be obtained from solutions of (8.14) by the transformation (8.13). Thus, we obtain a fundamental set $u_{1,2}(x; W)$ of solutions of (8.8):

$$\begin{aligned} &u_1(x; W) = \mathrm{e}^{-z/2}\Phi(\alpha, 1/2; z), \\ &u_2(x; W) = \mathrm{e}^{-z/2} x \Phi(\alpha + 1/2, 3/2; z), \ \ \overline{u_{1,2}(x; W)} = u_{1,2}(x; \overline{W}). \end{aligned} \tag{8.15}$$

The solutions $u_{1,2}(x; W)$ are real entire functions in W for any fixed x, and they form a special fundamental system of solutions of (8.8) for any υ and W, for which

$$u_k^{(l-1)}(0; W) = \delta_{kl}, \ k, l = 1, 2, \ \ \mathrm{Wr}(u_1, u_2) = 1\,.$$

Solutions (8.15) have the following asymptotics as $|x| \to \infty$ ($\alpha, \alpha + 1/2 \neq -n, \ n \in \mathbb{Z}_+$):

$$u_1(x; W) = \left[\frac{u(x; W)}{\Gamma(\tilde{\alpha})} + \frac{\overline{u(x; \overline{W})}}{\Gamma(\alpha)} \right] \tilde{O}(x^{-2}) = O\left(|x|^{-1/2 + 2|\operatorname{Im} w|} \right),$$

$$
\begin{aligned}
u_2(x;W) &= \pm\frac{1}{2\upsilon}\left[\frac{\mathrm{e}^{i\pi/4}u(x;W)}{\Gamma(\tilde{\alpha}+1/2)} + \frac{\mathrm{e}^{-i\pi/4}\overline{u(x;\overline{W})}}{\Gamma(\alpha+1/2)}\right]\tilde{O}(x^{-2}) \\
&= O(|x|^{-1/2+2|\operatorname{Im} w|}),\ \tilde{\alpha} = 1/4 - iw, \\
u(x;W) &= \sqrt{\pi}\mathrm{e}^{-i(\upsilon x)^2/2}(\mathrm{e}^{-i\pi/4}\upsilon|x|)^{-1/2-2iw}.
\end{aligned}
$$

Another fundamental system $v_{1,2}(x;W)$,

$$
\begin{aligned}
v_\pm(x;W) &= \frac{\mathrm{e}^{i\pi/4}}{\Gamma(\tilde{\alpha}+1/2)}u_1(x;W) \pm \frac{2\upsilon}{\Gamma(\tilde{\alpha})}u_2(x;W), \\
\mathrm{Wr}(v_+,v_-) &= -\frac{4\upsilon\mathrm{e}^{i\pi/4}}{\Gamma(\tilde{\alpha})\Gamma(\tilde{\alpha}+1/2)} = -\omega(W), \\
v_\pm(x;W) &= \begin{cases} O(|x|^{-1/2\pm 2\operatorname{Im} w}),\ x\to\infty, \\ O(|x|^{-1/2\mp 2\operatorname{Im} w}),\ x\to-\infty, \end{cases} \qquad \operatorname{Im} w > 0,
\end{aligned}
$$

of solutions of (8.8) (for $\alpha, \alpha + 1/2 \neq -n,\ n \in \mathbb{Z}_+$) is convenient (due to their asymptotic properties) to construct the Green's function.

These solutions are well defined for any υ and W, in particular for $\operatorname{Im} W > 0$, and are normalized as follows:

$$
v_\pm(0;W) = \mathrm{e}^{i\pi/4}\Gamma^{-1}(\tilde{\alpha}+1/2),\ \ v'_+(0;W) = -v'_-(0;W) = 2\upsilon\Gamma^{-1}(\tilde{\alpha}).
$$

The functions $v_\pm$ and their linear combinations are not square-integrable for $\operatorname{Im} W > 0$. The latter means that deficiency indices are zero, which confirms the fact that $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

In the standard manner, we obtain the Green's function

$$
G\,(x,y;W) = \omega^{-1}(W)\begin{cases} v_-(x;W)v_+(y;W),\ x > y, \\ v_+(x;W)v_-(y;W),\ x < y. \end{cases}
$$

Then following Sect. 5.3.2, we obtain the matrix function $M_{kl}(0;W)$,

$$
\begin{aligned}
M_{kl}(0;W) &= G_{kl}\,(-0,+0;W) = \operatorname{antidiag}(-1/2,1/2) \\
&\quad + \operatorname{diag}\left(\left[\mathrm{e}^{-2\pi w}+i\right]\rho_1(E), \left[-\mathrm{e}^{-2\pi w}+i\right]\rho_2(E)\right),\ E = \operatorname{Re} W, \\
\rho_1(E) &= \frac{1}{8\pi^2\upsilon}|\Gamma\left(1/4+iE/4\upsilon^2\right)|^2\mathrm{e}^{\pi E/4\upsilon^2}, \\
\rho_2(E) &= \frac{\upsilon}{2\pi^2}|\Gamma\left(3/4+iE/4\upsilon^2\right)|^2\mathrm{e}^{\pi E/4\upsilon^2},
\end{aligned}
$$

and the derivative of the matrix spectral function, $\sigma'_{kl}(E) = \operatorname{diag}(\rho_1(E),\rho_2(E))$.

Thus, the spectrum of $\hat{H}_1$ is twofold degenerate and reads spec $\hat{H}_1 = \mathbb{R}$. The eigenfunctions $U_{iE}(x) = \sqrt{\rho_i(E)}u_i(x;E)$, $i = 1,2$, $E \in \mathbb{R}$, of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R})$.

8.3 ESP III

In this case,

$$V(x) = g_1 x^{-1} + g_2 x^{-2}, \ \ x \in \mathbb{R}_+, \tag{8.16}$$

and the corresponding Schrödinger equation is

$$\psi'' - (g_1 x^{-1} + g_2 x^{-2} - W)\psi = 0\,. \tag{8.17}$$

The case $g_1 = 0$ corresponds to the Calogero potential and was already considered in Sect. 7.2, so that we keep $g_1 \neq 0$ in what follows.

It should be noted that on the physical level of rigor, the Schrödinger equation with potential (8.16) was studied for a long time in connection with different physical problems; see for example [61, 137] and books [59, 104]. The potential (8.16) is singular at the origin. It is repulsive at this point for $g_2 > 0$, and has a minimum at a point $x_0 > 0$ for $g_2 > 0$ and $g_1 > 0$. The potential with g_1, g_2 in the latter range is known as the *Kratzer potential* [100]. The Kratzer potential is conventionally used to describe molecular energy and structure, interactions between different molecules [22]. For $g_2 > 0$ and $g_1 > 0$, we have the inverse Kratzer potential, which is conventionally used to describe tunnel effects, scattering of charged particles [115] and decays, in particular, molecule ionization and fluorescence [19]. In addition, valence electrons in a hydrogen-like atom are described in terms of such a potential [54].

First we consider the case $g_2 \neq 0$ (the case $g_2 = 0$ is considered below in Sect. 8.3.5.

As in the previous cases, the initial symmetric operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}(\mathbb{R}_+)$ and $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$.

We first consider the Schrödinger equation (8.17). Introducing a new variable z and new functions $\phi_\pm$, instead of the respective x and $\psi(x)$,

$$z = \lambda x,\ \lambda = 2\sqrt{-W} = 2\sqrt{|W|}\mathrm{e}^{i(\varphi-\pi)/2},\ \psi(x) = x^{1/2\pm\mu}\mathrm{e}^{-z/2}\phi_\pm(z),$$

$$\mu = \begin{cases} \sqrt{g_2 + 1/4}, & g_2 \geq -1/4 \\ i\varkappa,\ \varkappa = \sqrt{|g_2| - 1/4}, & g_2 < -1/4 \end{cases},\ W = |W|\mathrm{e}^{i\varphi},\ 0 \leq \varphi \leq \pi, \tag{8.18}$$

we reduce (8.17) to the confluent hypergeometric equations for $\phi_\pm(z)$,

$$
\begin{aligned}
& z d_z^2 \phi_\pm(z) + (\beta_\pm - z) d_z \phi_\pm(z) - \alpha_\pm \phi_\pm(z) = 0, \\
& \alpha_\pm = 1/2 \pm \mu + g_1/\lambda, \ \beta_\pm = 1 \pm 2\mu,
\end{aligned} \tag{8.19}
$$

whose solutions are the known confluent hypergeometric functions $\Phi(\alpha_\pm, \beta_\pm; z)$ and $\Psi(\alpha_\pm, \beta_\pm; z)$; see [1, 20, 81].

Solutions $\psi(x)$ of (8.17) are restored from solutions of (8.19) by transformation (8.18). In what follows, we use $u_1(x; W)$, $u_2(x; W)$, and $\upsilon_1(x; W)$ defined by

$$
\begin{aligned}
u_1(x; W) &= x^{1/2+\mu} \mathrm{e}^{-z/2} \Phi(\alpha_+, \beta_+; z) = u_1(x; W)|_{\lambda \to -\lambda}, \\
u_2(x; W) &= x^{1/2-\mu} \mathrm{e}^{-z/2} \Phi(\alpha_-, \beta_-; z) = u_2(x; W)|_{\lambda \to -\lambda} \\
&= u_1(x; W)|_{\mu \to -\mu}, \ \upsilon_1(x; W) = \lambda^{2\mu} x^{1/2+\mu} \mathrm{e}^{-z/2} \Psi(\alpha_+, \beta_+; z) \\
&= \lambda^{2\mu} \frac{\Gamma(-2\mu)}{\Gamma(\alpha_-)} u_1 + \frac{\Gamma(2\mu)}{\Gamma(\alpha_+)} u_2.
\end{aligned} \tag{8.20}
$$

The function u_2 is not defined for $\beta_- = -n$, or $\mu = (n+1)/2, n \in \mathbb{Z}_+$, in particular, for $\mu = 1/2$. For such μ, we replace u_2 by other solutions of (8.17); they are considered in the subsequent sections.

The coefficients of the Taylor expansion of functions $u_1(x; W)/x^{1/2+\mu}$ and $u_2(x; W)/x^{1/2-\mu}$ with respect to x are polynomials in λ. Because these functions are even in λ, the coefficients are polynomials in W, whence it follows that $u_1(x; W)$ and $u_2(x; W)$ are entire functions in W at any point x except $x = 0$ for u_2 with $\mu > 1/2$.

If $g_2 \geq -1/4$ $(\mu \geq 0)$, then $u_1(x; W)$ and $u_2(x; W)$ are real entire functions of W. If $g_2 < -1/4$ $(\mu = i\varkappa)$, then $u_2(x; E) = \overline{u_1(x; E)}$.

The pairs u_1, u_2 with $\mu \neq 0$ and u_1, υ_1 for $\operatorname{Im} W \neq 0$ are the fundamental systems of solutions of (8.17) because the respective Wronskians are

$$
\mathrm{Wr}(u_1, u_2) = -2\mu, \ \mathrm{Wr}(u_1, \upsilon_1) = -\Gamma(\beta_+)/\Gamma(\alpha_+) \equiv -\omega(W). \tag{8.21}
$$

The well-known asymptotics of the special functions Φ and Ψ, see e.g. [20], entering solutions (8.20) allow us to estimate simply the asymptotic behavior of the solutions at the origin as $x \to 0$, and at infinity as $x \to \infty$.

As $x \to 0$, we have

$$
\begin{aligned}
& u_1(x; W) = \kappa_0^{-1/2-\mu} u_{1\mathrm{as}}(x) + O(x^{3/2+\mu}), \ u_2(x; W) = \kappa_0^{-1/2+\mu} u_{2\mathrm{as}}(x) \\
& \quad + \begin{cases} O(x^{5/2-\mu}), \ -1/4 < g_2 < 3/4, \ g_2 \neq 0, \\ (0 < \mu < 1, \ \mu \neq 1/2), \\ O(x^{3/2}), \ g_2 < -1/4 \ (\mu = i\varkappa), \end{cases}
\end{aligned} \tag{8.22}
$$

and if $\alpha_+ \neq -n, \alpha_- \neq -m, \ n, m \in \mathbb{Z}_+$,

$$
\upsilon_1(x;W) = \begin{cases} \frac{\Gamma(2\mu)}{\Gamma(\alpha_+)} x^{1/2-\mu}\tilde{O}(x),\ g_2 \geq 3/4\ (\mu \geq 1), \\ \frac{\lambda^{2\mu}\Gamma(-2\mu)}{\Gamma(\alpha_-)}\kappa_0^{-1/2-\mu} u_{1\mathrm{as}}(x) + \frac{\Gamma(2\mu)}{\Gamma(\alpha_+)}\kappa_0^{-1/2+\mu} u_{2\mathrm{as}}(x), \\ +O(x^{3/2}),\ -1/4 < g_2 < 3/4,\ g_2 \neq 0\ (0 < \mu < 1,\ \mu \neq 1/2), \\ \frac{\lambda^{2i\varkappa}\Gamma(-2i\varkappa)}{\Gamma(\alpha_-)}\kappa_0^{-1/2-i\varkappa} u_{1\mathrm{as}}(x) + \frac{\Gamma(2i\varkappa)}{\Gamma(\alpha_+)}\kappa_0^{-1/2+i\varkappa} u_{2\mathrm{as}}(x), \\ +O(x^{3/2}),\ g_2 < -1/4\ (\mu = i\varkappa), \end{cases} \tag{8.23}
$$

where

$$
u_{1\mathrm{as}}(x) = (\kappa_0 x)^{1/2+\mu},
$$

$$
u_{2\mathrm{as}}(x) = \begin{cases} (\kappa_0 x)^{1/2-\mu} - \frac{g_1/\kappa_0}{2\mu-1}(\kappa_0 x)^{3/2-\mu},\ -1/4 < g_2 < 3/4,\ g_2 \neq 0, \\ (0 < \mu < 1,\ \mu \neq 1/2), \\ (\kappa_0 x)^{1/2-i\varkappa},\ g_2 < -1/4\ (\mu = i\varkappa), \end{cases}
$$

and κ_0 is an arbitrary, but fixed, parameter of dimension of inverse length.

As $x \to \infty,\ \operatorname{Im} W > 0$, we have

$$
\begin{aligned} u_1(x;W) &= \frac{\Gamma(\beta_+)}{\Gamma(\alpha_+)}\lambda^{\alpha_+-\beta_+} x^{g_1/\lambda} \mathrm{e}^{z/2}\tilde{O}(x^{-1}) \\ &= O\left(x^a \mathrm{e}^{|W|^{1/2}\sin(\varphi/2)}\right),\ \upsilon_1(x;W) = \lambda^{-\alpha_-} x^{-g_1/\lambda}\mathrm{e}^{-z/2}\tilde{O}(x^{-1}) \\ &= O\left(x^{-a}\mathrm{e}^{-|W|^{1/2}\sin(\varphi/2)}\right),\ a = 2^{-1}|W|^{-1/2} g_1 \sin(\varphi/2)\,. \end{aligned}
$$

The obtained asymptotics are sufficient to allow definite conclusions about the deficiency indices of the initial symmetric operator $\hat{H}$ as functions of the parameters g_1, g_2 and thereby about a possible variety of its s.a. extensions. It is evident that for Im > 0, the function $u_1(x;W)$ exponentially increasing at infinity is not square-integrable. The function $\upsilon_1\ (x;W)$ exponentially decreasing at infinity is not square-integrable at the origin for $g_2 \geq 3/4$ $(\mu \geq 1)$, whereas for $g_2 < 3/4$, it is (moreover, for $g_2 < 3/4$, any solution of (8.17) is square-integrable at the origin). Because for $\operatorname{Im} W > 0$, the functions u_1, υ_1 form a fundamental system of (8.17), this equation with $\operatorname{Im} W > 0$ has no square-integrable solutions for $g_2 \geq 3/4$, whereas for $g_2 < 3/4$, there exists one square-integrable solution, $\upsilon_1\ (x;W)$. This means that the deficiency indices of the initial symmetric operator $\hat{H}$ are equal to zero for $g_2 \geq 3/4$, and are $m_\pm = 1$ for $g_2 < 3/4$.

Analogously, for $g_2 \geq 3/4$, there is a unique s.a. extension of $\hat{H}$, whereas for $g_2 < 3/4$, there exists a one-parameter family of s.a. extensions of $\hat{H}$. A structure of these extensions, in particular an appearance of their specifying asymptotic boundary conditions, depends crucially on a specific range of values of the parameter g_2. In what follows, we distinguish five such regions and consider them separately.

8.3.1 Range 1

In this range, we have

$$g_2 \geq 3/4 \ (\mu \geq 1)\,. \tag{8.24}$$

As was mentioned above, the deficiency indices of the initial symmetric operator $\hat{H}$ with g_2 in this range are zero. This implies that for $g_2 \geq 3/4$, the operator $\hat{H}^+$ is s.a. and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$ with the domain $D_{H_1} = D^*_{\check{H}}(\mathbb{R}_+)$.

A spectral analysis of the s.a. operator $\hat{H}_1 = \hat{H}^+$ begins with an evaluation of its Green's function $G(x, y; W)$, which is the kernel of the integral representation of the solution $\psi_*(x)$ of the inhomogeneous differential equation

$$\left(\check{H} - W\right)\psi_*(x) = \eta(x),\ \ \eta(x) \in L^2(\mathbb{R}_+) \tag{8.25}$$

with $\operatorname{Im} W \neq 0$ under the condition that $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$. The general solution of this equation without the condition of square-integrability can be represented as

$$\begin{aligned} \psi_*(x) &= a_1 u_1(x; W) + a_2 \upsilon_1(x; W) + I(x; W), \\ \psi_*'(x) &= a_1 u_1'(x; W) + a_2 \upsilon_1'(x; W) + I'(x; W), \end{aligned} \tag{8.26}$$

where

$$\begin{aligned} I(x; W) &= \int_0^x G^{(+)}(x, y; W)\,\eta(y)\mathrm{d}y + \int_x^\infty G^{(-)}(x, y; W)\,\eta(y)\mathrm{d}y, \\ I'(x; W) &= \int_0^x d_x G^{(+)}(x, y; W)\,\eta(y)\mathrm{d}y + \int_x^\infty d_x G^{(-)}(x, y; W)\,\eta(y)\mathrm{d}y, \\ G^{(+)}(x, y; W) &= \omega^{-1}(W)\upsilon_1(x; W)u_1(y; W), \\ G^{(-)}(x, y; W) &= \omega^{-1}(W)u_1(x; W)\upsilon_1(y; W), \end{aligned}$$

with ω given in (8.21). Using the Cauchy–Schwarz inequality, it is easy to show that $I(x; W)$ is bounded as $x \to \infty$. The condition $\psi_*(x) \in L^2(\mathbb{R}_+)$ then implies that $a_1 = 0$, because $u_1(x; W)$ exponentially grows while $\upsilon_1(x; W)$ exponentially decreases at infinity. As $x \to 0$, we have $I(x) \sim O(x^{3/2})$, $I'(x) \sim O(x^{1/2})$ (up to logarithmic accuracy at $g_2 = 3/4$), whereas $\upsilon_1(x; W)$ is not square-integrable at the origin. The condition $\psi_*(x) \in L^2(\mathbb{R}_+)$ then implies that $a_2 = 0$. In addition, we see that the asymptotic behavior of functions $\psi_*(x)$ belonging to $D^*_{\check{H}}(\mathbb{R}_+)$ at the origin, as $x \to 0$, is estimated by

$$\psi_*(x) = O(x^{3/2}),\ \psi_*'(x) = O(x^{1/2}).$$

Together with the fact that the functions ψ_* vanish at infinity (see below), this implies that the asymmetry form Δ_{H^+} is trivial, which confirms that in the first range, the operator $\hat{H}^+$ is symmetric and therefore s.a. (in contrast to the next ranges considered in the subsequent sections).

It follows that the Green's function of $\hat{H}_1$ is given by

$$G\left(x, y; W\right) = \begin{cases} G^{(+)}\left(x, y; W\right), & x > y, \\ G^{(-)}\left(x, y; W\right), & x < y. \end{cases}$$

The representation (8.20) of the function υ_1 in terms of the functions u_1 and u_2 is inconvenient sometimes because the individual summands do not exist for some μ although υ_1 does. For our purposes, other representations are convenient. For $m - 1 < 2\mu < m + 1$, $m \geq 2$, the function $\upsilon_1(x; W)$ can be represented as

$$\begin{aligned}
\upsilon_1(x; W) &= A_m(W)u_1(x; W) + \frac{\omega(W)}{2\mu}\upsilon_{(m)}(x; W), \\
A_m(W) &= \lambda^{2\mu}\frac{\Gamma(-2\mu)}{\Gamma(\alpha_-)} + a_m(W)\frac{\Gamma(2\mu)\Gamma(\beta_-)}{\Gamma(\alpha_+)}, \\
\upsilon_{(m)}(x; W) &= u_2\left(x; W\right) - a_m(W)\Gamma(\beta_-)u_1\left(x; W\right), \\
a_m(W) &= \lambda^m\frac{\Gamma(\alpha_{+m})}{m!\Gamma(\alpha_{-m})},\ \alpha_{\pm m} = \frac{1 \pm m}{2} + g_1/\lambda.
\end{aligned}$$

It is easy to see that all the coefficients $a_m(W)$ are polynomials in W that are real for $\operatorname{Im} W = 0$ ($W = E$). In view of the relation

$$\lim_{\beta \to -n} \Gamma^{-1}(\beta)\Phi(\alpha, \beta; x) = \frac{x^{n+1}\Gamma(\alpha + n + 1)}{(n+1)!\Gamma(\alpha)}\Phi(\alpha + n + 1, n + 2; x) \quad (8.27)$$

(see [20, 81]), the functions $\upsilon_{(m)}(x; W)$ and $A_m(W)$ exist for $m - 1 < 2\mu < m + 1$ and for any W. In fact, $\upsilon_{(m)}(x; W)$ are particular solutions of (8.17) that are real entire in W and have the properties (for $m - 1 < 2\mu < m + 1$)

$$\operatorname{Wr}(u_1, \upsilon_{(m)}) = -2\mu,\ \upsilon_{(m)}(x; W) = x^{1/2-\mu}\tilde{O}(x),\ x \to 0.$$

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty u_1(x; W)\xi(x)\mathrm{d}x,\ \xi \in D_r(\mathbb{R}_+) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ ($\tilde{U} = V_{(m)}$), and therefore, the spectrum of $\hat{H}_1$ is simple.

The derivative of the spectral function is given by

$$\sigma'(E) = \pi^{-1}\,\mathrm{Im}\left[\omega^{-1}(E+i0)A_m(E+i0)\right]. \tag{8.28}$$

Because $\omega^{-1}(W)A_m(W)$ is an analytic function of μ, its value at $\mu = m/2$ is a limit as $\mu \to m/2$. For $\mu \neq m/2$, representation (8.28) can be simplified to

$$\sigma'(E) = \mathrm{Im}\,\Omega^{-1}(E+i0),\ \ \Omega(W) = \frac{\pi\Gamma(\alpha_-)\Gamma(\beta_+)}{\lambda^{2\mu}\Gamma(-2\mu)\Gamma(\alpha_+)}\,.$$

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we obtain

$$\sigma'(E) = \left(\frac{|\Gamma(\alpha_+)|}{\Gamma(\beta_+)}\right)^2 \frac{(2p)^{2\mu}\mathrm{e}^{-\pi g_1/2p}}{2\pi} > 0.$$

We see that $\sigma'(E)$ is a nonsingular function for $E \geq 0$. It follows that the spectrum of the s.a. Hamiltonian $\hat{H}_1$ is continuous for all such values of E.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega^{-1}(E)$ is real for all values of E where $\Omega^{-1}(E)$ is finite, which implies that $\mathrm{Im}\,\Omega^{-1}(E+i0)$ can differ from zero only at the discrete points E_n where $\Omega(E_n) = 0$. It is easy to see that the latter equation is reduced to the equations $\alpha_+(E_n) = -n$, $n \in \mathbb{Z}_+$, which have solutions only if $g_1 < 0$, and the solutions E_n are then given by

$$E_n = -g_1^2(1+2\mu+2n)^{-2},\ \ \tau_n = |g_1|\,(1+2\mu+2n)^{-1}\,. \tag{8.29}$$

We thus obtain that for $E < 0$, the function $\sigma'(E)$ is equal to zero if $g_1 > 0$, whereas if $g_1 < 0$, this function is given by

$$\sigma'(E) = \sum_{n=0}^{\infty} Q_n^2\delta(E-E_n),\ \ Q_n = \frac{(2\tau_n)^{\mu+1}}{\Gamma(\beta_+)}\sqrt{\frac{\Gamma(1+2\mu+n)}{(1+2\mu+2n)\,n!}}.$$

The final result of this section is as follows. For $g_2 > 3/4$, the spectrum of $\hat{H}_1$ is simple and given by

$$\mathrm{spec}\ \hat{H}_1 = \begin{cases} \mathbb{R}_+,\ g_1 > 0, \\ \mathbb{R}_+ \cup \{E_n,\},\ g_1 < 0. \end{cases}$$

For $g_1 > 0$, the generalized eigenfunctions $U_E\,(x) = \sqrt{\sigma'(E)}u_1(x;E)$, $E \geq 0$, of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. For $g_1 < 0$, the generalized eigenfunctions $U_E\,(x) = \sqrt{\sigma'(E)}u_1(x;E)$, $E \geq 0$, of $\hat{H}_1$ together with the eigenfunctions $U_n(x) = Q_n u_1(x;E_n)$, $n \in \mathbb{Z}_+$, form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

8.3.2 Range 2

In this range, we have

$$\frac{3}{4} > g_2 > -\frac{1}{4}\ (1 > \mu > 0).$$

To obtain asymptotics of functions from $D^*_{\check{H}}(\mathbb{R}_+)$, we consider the general solution of (8.25). Because in the range under consideration, any solution of (8.17) is square-integrable at the origin, the general solution of (8.25) with $W = 0$ can be represented as

$$\psi_*(x) = a_1 u_1(x;0) + a_2 u_2(x;0) \\ -\frac{1}{2\mu}\int_0^x \left[u_1(x;0)u_2(y;0) - u_2(x;0)u_1(y;0)\right]\eta(y)\mathrm{d}y. \quad (8.30)$$

It follows from Lemma 2.14 that $\psi_*(x), \psi_*'(x) \overset{x\to\infty}{\longrightarrow} 0$ because the corresponding potential tends to zero as $x \to \infty$.

The asymptotic behavior of integral terms in (8.30) as $x \to 0$ is estimated with the help of the Cauchy–Schwarz inequality, and we obtain

$$\psi_*(x) = a_1 u_{1\mathrm{as}}(x) + a_2 u_{2\mathrm{as}}(x) + O\left(x^{3/2}\right),$$
$$\psi_*'(x) = a_1 u_{1\mathrm{as}}'(x) + a_2 u_{2\mathrm{as}}'(x) + O\left(x^{1/2}\right).$$

Taking into account the asymptotic behavior of functions (8.30) as $x \to 0$ and $x \to \infty$, we obtain $\Delta_{H^+}(\xi) = -2\mu k_0(\overline{a_1}a_2 - \overline{a_2}a_1)$. Such a structure implies that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. Imposing the condition $\Delta_{H^+}(\xi) = 0$, we obtain a relation on the coefficients a_1 and a_2,

$$a_2 \sin\nu = a_1 \cos\nu,\ \nu \in \mathbb{S}\left(-\pi/2, \pi/2\right).$$

Thus, in the range under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{2,\nu}$ parameterized by ν with domains $D_{H_{2,\nu}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior at the origin $x \to 0$:

$$\psi(x) = C\psi^{\mathrm{as}}(x) + O(x^{3/2}),\ \psi'(x) = C\psi^{\mathrm{as}\prime}(x) + O(x^{1/2}),$$
$$\psi^{\mathrm{as}}(x) = u_{1\mathrm{as}}(k_0 x)\sin\nu + u_{2\mathrm{as}}(x,k_0)\cos\nu. \quad (8.31)$$

Imposing boundary condition (8.31) on the function (8.26) (with $a_1 = 0$), and using asymptotics (8.22) and (8.23), we obtain Green's functions of the operators $\hat{H}_{2,\nu}$:

$$G(x,y;W) = \Omega^{-1}(W)u_{2,\nu}(x;W)u_{2,\nu}(y;W) \\ +\frac{1}{2\mu k_0}\begin{cases} \tilde{u}_{2,\nu}(x;W)u_{2,\nu}(y;W),\ x > y, \\ u_{2,\nu}(x;W)\tilde{u}_{2,\nu}(y;W),\ x < y, \end{cases} \quad (8.32)$$

where

$$
\begin{aligned}
u_{2,\nu}(x;W) &= k_0^{1/2+\mu}u_1(x;W)\sin\nu + k_0^{1/2-\mu}u_2(x;W)\cos\nu,\\
\tilde{u}_{2,\nu}(x;W) &= -k_0^{1/2+\mu}u_1(x;W)\cos\nu + k_0^{1/2-\mu}u_2(x;W)\sin\nu,\\
\Omega(W) &= 2\mu k_0\omega_2(W)\tilde{\omega}_2^{-1}(W),\\
\omega_2(W) &= \sin\nu + f(W)\cos\nu,\ \tilde{\omega}_2(W) = \cos\nu - f(W)\sin\nu,\\
f(W) &= (\lambda/k_0)^{2\mu}\frac{\Gamma(\alpha_+)\Gamma(\beta_-)}{\Gamma(\alpha_-)\Gamma(\beta_+)},
\end{aligned}
$$

and we used the relation

$$
v_1(x;W) = (2\mu)^{-1}k_0^{-1/2+\mu}\omega(W)[\tilde{\omega}_{2,\nu}(W)u_{2,\nu}(x;W) + \omega_{2,\nu}(W)\tilde{u}_{2,\nu}(x;W)].
$$

We note that the functions $u_{2,\nu}(x;W)$ and $\tilde{u}_{2,\nu}(x;W)$ are solutions of (8.17) that are real entire in W, $u_{2,\nu}(x;W)$ satisfies boundary condition (8.31), and the second summand on the right-hand side of (8.32) is real for real $W = E$.

Consider the guiding functional

$$
\Phi(\xi;W) = \int_0^\infty u_{2,\nu}(x;W)\xi(x)\mathrm{d}x,\ \xi \in \mathbb{D} = D_r(\mathbb{R}_+)\cap D_{H_{2,\nu}}.
$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{2,\nu}$ ($\tilde{U} = \tilde{u}_{2,\nu}$), and therefore, the spectra of $\hat{H}_{2,\nu}$ are simple. The derivative of the spectral function reads $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E+i0)$.

It is convenient to consider the cases $|\nu| < \pi/2$ and $\nu = \pm\pi/2$ separately. We first consider the case $\nu = \pi/2$, where we have

$$
u_{2,\pi/2}(x;W) = k_0^{1/2+\mu}u_1(x;W),\ \Omega^{-1}(W) = -\frac{\Gamma(\alpha_+)\Gamma(\beta_-)(\lambda/k_0)^{2\mu}}{2\mu k_0\Gamma(\alpha_-)\Gamma(\beta_+)}.
$$

We see that all results for spectrum and system of the normalized (generalized) eigenfunctions coincide with those of the first range ($g_2 \geq 3/4$). In particular, the expressions for discrete energy levels (we will denote them by $\mathcal{E}_n$) are given by (8.29):

$$
\mathcal{E}_n = -\frac{g_1^2}{(1+2\mu+2n)^2},\ \tau_n = \sqrt{|\mathcal{E}_n|} = \frac{|g_1|}{1+2\mu+2n}.
$$

We obtain the same results in the case $\nu = -\pi/2$.

Second, we consider the case $\nu = 0$. Here we have

$$
\begin{aligned}
&u_{2,0}(x;W) = k_0^{1/2-\mu}u_2(x;W),\\
&\qquad \sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E+i0),\ \Omega^{-1}(W) = \frac{(k_0/\lambda)^{2\mu}\Gamma(\beta_+)\Gamma(\alpha_-)}{2\mu k_0\Gamma(\beta_-)\Gamma(\alpha_+)}.
\end{aligned}
$$

Let $g_1 > 0$. For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we have

$$\sigma'(E) = \left(\frac{|\Gamma(\alpha_-)|}{|\Gamma(\beta_-)|}\right)^2 \frac{(k_0/2p)^{2\mu}\mathrm{e}^{-\pi g_1/2p}}{2\pi k_0}. \tag{8.33}$$

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega^{-1}(E)$ is real for those E for which $\Omega^{-1}(E)$ is finite, so that $\mathrm{Im}\,\Omega^{-1}(E + i0)$ can differ from zero only for E that provide $\Omega^{-1}(E) = \infty$. The latter is possible only for $\alpha_- = -n$ ($\Gamma(\alpha_-) = \infty$), $n \in \mathbb{Z}_+$, or

$$1 - 2\mu + g_1/\tau = -2n, \; n \in \mathbb{Z}_+. \tag{8.34}$$

Equations (8.34) have no solutions for $0 < \mu < 1/2$ and have one solution for $1/2 < \mu < 1$: $n = 0$, $\tau = \tau_{-1}(0) = g_1/(2\mu - 1)$, $E = E_{-1}(0) = -\tau_{-1}^2(0)$.

Let $g_1 < 0$. For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, the derivative of the spectral function is given by (8.33).

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega^{-1}(E)$ is real for $E \neq E_n(0)$ ($\Omega(E_n(0)) = \infty$), so that $\sigma'(E)$ does not vanish only at the points $E = E_n(0)$. The equation $\Omega^{-1}(E_n(0)) = \infty$ implies the condition $\alpha_- = 1/2 - \mu - |g_1|/2\tau_n(0) = -n$ ($\Gamma(\alpha_-) = \infty$), which gives

$$E_n(0) = -\tau_n^2(0) = -\left(\frac{g_1}{1 - 2\mu + 2k}\right)^2, \; k = \begin{cases} n, & 0 < \mu < 1/2, \\ n + 1, & 1/2 < \mu < 1, \end{cases} \quad n \in \mathbb{Z}_+.$$

Thus for $g_1 < 0$, the simple spectrum of $\hat{H}_{2,0}$ is given by spec $H_{2,0} = \mathbb{R}_+ \cup \{E_n(0), \; n \in \mathbb{Z}_+\}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of (generalized) eigenfunctions

$$\begin{aligned} U_E(x) &= \sqrt{\sigma'(E)}u_2(x; E), \; E \geq 0, \\ U_n(x) &= \frac{(2\tau_n)^{1-\mu}}{|\Gamma(\beta_-)|}\sqrt{\frac{\Gamma(1 - 2\mu + k)}{(1 - 2\mu + 2k)k!}}u_2(x; E_n(0)), \; n \in \mathbb{Z}_+, \end{aligned} \tag{8.35}$$

of $\hat{H}_{2,0}$.

For $0 < \mu < 1/2$, $g_1 > 0$, the simple spectrum of $\hat{H}_{2,0}$ is given by spec $\hat{H}_{2,0} = \mathbb{R}_+$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of generalized eigenfunctions $U_E(x)$ (8.35) with the corresponding parameters and the function $\sigma'(E)$.

For $1/2 < \mu < 1$, $g_1 > 0$, the simple spectrum of $\hat{H}_{2,0}$ is given by spec $H_{2,0} = \mathbb{R}_+ \cup \{E_{-1}(0)\}$ and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ consists of generalized eigenfunctions $U_E(x)$ (8.35) with the corresponding parameters and the function $\sigma'(E)$, and only one eigenfunction of the discrete spectrum $U_{-1}(x)$, given by (8.35) with $n = -1$ and $k = 0$.

Now we turn to the general case $|\nu| < \pi/2$. In this case we have

$$\sigma'(E) = \left(2\pi\mu k_0 \cos^2\nu\right)^{-1} \operatorname{Im} f_\nu^{-1}(E + i0),$$

$$f_\nu(W) = f(W) + \tan\nu,\ f(W) = \frac{(\lambda/k_0)^{2\mu}\Gamma(\beta_-)\Gamma(\alpha_+)}{\Gamma(\beta_+)\Gamma(\alpha_-)}.$$

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we have

$$\sigma'(E) = \frac{B(E)}{2\pi k_0 \cos^2\nu[A^2(E) + \mu^2 B^2(E)]}, \tag{8.36}$$

where $A(E) = \operatorname{Re} f_\nu(E)$ and $\mu B(E) = -\operatorname{Im} f_\nu(E)$. A direct calculation gives

$$A(E) = \frac{\mu|\Gamma(\alpha_+)|^2(2p/k_0)^{2\mu}}{\sin(2\pi\mu)\Gamma^2(\beta_+)}\left(\mathrm{e}^{-\pi g_1/2p}\cos(2\pi\mu) + \mathrm{e}^{\pi g_1/2p}\right) + \tan\nu,$$

$$B(E) = \frac{|\Gamma(\alpha_+)|^2(2p/k_0)^{2\mu}\mathrm{e}^{-\pi g_1/2p}}{\Gamma^2(\beta)}\ . \tag{8.37}$$

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $f_\nu(E)$ is real, and therefore, $\sigma'(E)$ can differ from zero only at the discrete points $E_n(\nu)$ such that $f_\nu(E_n(\nu))=0$, or $f(E_n(\nu)) = -\tan\nu$, and we obtain that

$$\sigma'(E) = \sum_n \left[-2\mu k_0 f_\nu'(E_n(\nu))\cos^2\nu\right]^{-1}\delta(E - E_n(\nu)),$$

$$f_\nu'(E_n(\nu)) = f'(E_n(\nu)) < 0,\ \partial_\nu E_n(\nu) = -\cos^{-2}\nu\left[f'(E_n(\nu))\right]^{-1} > 0. \tag{8.38}$$

1. Let $g_1 > 0$. For $E = p^2 > 0$, $p > 0$, the function $\sigma'(E)$ (8.36) is a finite positive function. At $E = 0$, we have $B(0) = 0$ and

$$A(0)|_{\nu=\nu_{-1}} = 0,\ \tan\nu_{-1} = -\frac{(g_1/k_0)^{2\mu}\Gamma(\beta_-)}{\Gamma^{-1}(\beta_+)},\ \begin{cases}\nu_{-1} > 0,\ 1/2 < \mu < 1,\\ \nu_{-1} < 0,\ 0 < \mu < 1/2.\end{cases}$$

It is easy to see that

$$f_\nu(W) = \tan\nu - \tan\nu_{-1} - \left(2\mu k_0\cos^2\nu_{-1}\right)^{-1}\Psi^{-2}W + O(W),\ W \to 0\,,$$

$$\Psi = \frac{g_1(g_1/k_0)^{-\mu}}{\mu\cos\nu_{-1}}\sqrt{\frac{3\Gamma(1+2\mu)}{2k_0(1+2\mu)\Gamma(2-2\mu)}}.$$

It follows that for $\nu \neq \nu_{-1}$, the function $\sigma'(E)$ is finite at $E = 0$. But for $\nu = \nu_{-1}$ and for small E, we have

$$\sigma'(E) = -\frac{1}{\pi}\Psi^2\operatorname{Im}(E + i0)^{-1} + O(1) = \Psi^2\delta(E) + O(1),$$

which means that there is the eigenvalue $E = 0$ in the spectrum of the s.a. Hamiltonian $\hat{H}_{2,\nu_{-1}}$.

For $E = -\tau^2 < 0$, $\lambda = 2\tau$, the function $f(E)$,

$$f(E) = \frac{\Gamma(\beta_-)}{\Gamma(\beta_+)} \frac{\Gamma(1/2 + \mu + g_1/2\tau)(2\tau/k_0)^{2\mu}}{\Gamma(1/2 - \mu + g_1/2\tau)},$$

has the properties that $f(E)$ is a smooth function for $E \in (-\infty, 0)$, $f(E) \to \infty$ as $E = -\infty$,

$$f(0) = -\tan \nu_{-1} \begin{cases} < 0, \ 1/2 < \mu < 1, \\ > 0, \ 0 < \mu < 1/2. \end{cases}$$

Because $f'(E_n(\nu)) < 0$, the straight line $\tilde{f}(E) = -\tan \nu$, $E \in (-\infty, 0]$, can intersect the plot of the function $f(E)$ no more than once. That is why the equation $f_\nu(E) = 0$ has no solutions for $\nu \in (\nu_{-1}, \pi/2)$, while for any fixed $\nu \in (-\pi/2, \nu_{-1}]$, this equation has only one solution $E_{-1}(\nu) \in (-\infty, 0]$, which increases monotonically from $-\infty$ to 0 as ν changes from $-\pi/2 + 0$ to ν_{-1}.

We thus obtain that the spectrum of $\hat{H}_{2,\nu}$, $|\nu| < \pi/2$, with $g_1 > 0$ is simple and given by

$$\operatorname{spec} \hat{H}_{2,\nu} = \begin{cases} \mathbb{R}_+ \cup \{E_{-1}(\nu)\}, \ \nu \in (-\pi/2, \nu_{-1}], \\ \mathbb{R}_+, \ \nu \in (\nu_{-1}, \pi/2). \end{cases}$$

The generalized eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,\nu}(x; E), \ E \geq 0,$$

and (for $\nu \in (-\pi/2, \nu_{-1}]$) the eigenfunction

$$U_{-1}(x) = \left[-2\mu k_0 f'(E_{-1}(\nu)) \cos^2 \nu\right]^{-1/2} u_{2,\nu}(x; E_{-1}(\nu))$$

of $\hat{H}_{2,\nu}$, form a complete orthonormalized systems in $L^2(\mathbb{R}_+)$.

2. Let $g_1 < 0$. Then for $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2pe^{-i\pi/2}$, formulas (8.36) and (8.37) hold. Because the functions $A(E)$ and $B(E)$ are finite at $E = 0$ ($B(0) \neq 0$), the function $\sigma'(E)$ (8.36) is a finite positive function for $E \geq 0$. This means that for $E \geq 0$, the spectra of s.a. Hamiltonians $\hat{H}_{2,\nu}$ are simple, purely continuous, and given by spec $\hat{H}_{2,\nu} = \mathbb{R}_+$.

   For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, we have

$$f(E) = \frac{\Gamma(\beta_-)}{\Gamma(\beta_+)} \frac{\Gamma(1/2 + \mu - |g_1|/2\tau)(2\tau/k_0)^{2\mu}}{\Gamma(1/2 - \mu - |g_1|/2\tau)}.$$

It is easy to see that for fixed ν, the spectrum is bounded from below and the equation $f_\nu(E_n(\nu)) = 0$ has an infinite number of solutions,

$$E_n(\nu) = -g_1^2/4n^2 + O(n^{-3}),$$

asymptotically coinciding with (8.29) as $n \to \infty$.

We thus obtain that the spectrum of $\hat{H}_{2,\nu}$, $|\nu| < \pi/2$, with $g_1 < 0$ is simple and given by spec $\hat{H}_{2,\nu} = \mathbb{R}_+ \cup \{E_n(\nu)\}$. The corresponding generalized eigenfunctions of the continuous spectrum

$$U_E(x) = \sqrt{\sigma'(E)} u_{2,\nu}(x; E), \; E \geq 0,$$

and eigenfunctions of the discrete spectrum

$$U_n(x) = \left[-2\mu k_0 f'(E_n(\nu)) \cos^2 \nu\right]^{-1/2} u_{2,\nu}(x; E_n(\nu)), \; E_n(\nu) < 0,$$

of $\hat{H}_{2,\nu}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

It is possible to give a description of the discrete spectrum of the Hamiltonians $\hat{H}_{2,\nu}$, $|\nu| < \pi/2$, $g_1 < 0$, in more detail.

The function $f(E)$ has the properties $f(E) \to \infty$ as $E \to -\infty$; $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n \in \mathbb{Z}_+$, and we have

$$E_n(0) < \mathcal{E}_n < E_{n+1}(0) < \mathcal{E}_{n+1}, \; n \in \mathbb{Z}_+.$$

Taking the second equality in (8.38) into account, we can see that in each energy interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, for a fixed $\nu \in (-\pi/2, \pi/2)$, there is one discrete level $E_n(\nu)$ that increases monotonically from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ when ν changes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $\mathcal{E}_{-1} = -\infty$). We note that the relations

$$\lim_{\nu \to \pi/2} E_n(\nu) = \lim_{\nu \to -\pi/2} E_{n+1}(\nu) = \mathcal{E}_n, \; n \in \mathbb{Z}_+,$$

confirm the equivalence of s.a. extensions with parameters $\nu = -\pi/2$ and $\nu = \pi/2$.

It should be also pointed out that bound states exist even for the repulsive potential, g_2,$g_1 > 0$.

8.3.3 Range 3

In this range, we have

$$g_2 = -1/4 \; (\mu = 0).$$

The analysis in this section is similar to that in the previous section. A peculiarity is that $\alpha_+ = \alpha_- = \alpha = 1/2 + g_1/\lambda$, $\beta_+ = \beta_- = 1$, $u_1(x; W) = u_2(x; W)$, and representation (8.20) of $\upsilon_1(x; W)$ in terms of u_1 and u_2 does not hold. As the solutions of (8.17) with $g_2 = -1/4$, we therefore use the functions $u_1(x; W)$, $u_3(x; W)$, and $\upsilon_1(x; W)$ respectively defined by

$$
\begin{aligned}
&u_1(x;W) = x^{1/2}\mathrm{e}^{-z/2}\Phi(\alpha,1;z) = u_1(x;W)|_{\lambda\to-\lambda},\\
&u_3(x;W) = \frac{\partial}{\partial\mu}\left[u_1(x;W)|_{\mu\neq 0}\right]_{\mu=0} + \ln k_0 u_1(x;W),\\
&v_1(x;W) = x^{1/2}\mathrm{e}^{-z/2}\Psi(\alpha,1;z) = \Gamma^{-1}(\alpha)\left[\omega_0(W)u_1(x;W) - u_3(x;W)\right],\\
&\quad \omega_0(W) = 2\psi(1) - \psi(\alpha) - \ln(\lambda/k_0),
\end{aligned}
$$

where $\psi(\alpha) = \Gamma'(\alpha)/\Gamma(\alpha)$ and k_0 is a constant. The functions $u_1(x;W)$ and $u_3(x;W)$ are real entire in W.

The asymptotic behavior of these functions at the origin and at infinity is respectively as follows.

As $x \to 0$, $z = \lambda x \to 0$, we have

$$
\begin{aligned}
&u_1(x;W) = k_0^{-1/2}u_{1\mathrm{as}}(x) + O(x^{3/2}),\ \ u_{1\mathrm{as}}(x) = (k_0x)^{1/2},\\
&u_3(x;W) = k_0^{-1/2}u_{3\mathrm{as}}(x) + O(x^{3/2}\ln x),\ \ u_{3\mathrm{as}}(x) = (k_0x)^{1/2}\ln(k_0x),\\
&v_1(x;W) = k_0^{-1/2}\Gamma^{-1}(\alpha)\left[\omega_0(W)u_{1\mathrm{as}}(x) - u_{3\mathrm{as}}(x)\right] + O(x^{3/2}\ln x).
\end{aligned} \tag{8.39}
$$

As $x \to \infty$, $\operatorname{Im} W > 0$, we have

$$
\begin{aligned}
&u_1(x;W) = \Gamma^{-1}(\alpha)\lambda^{\alpha-1}x^{g_1/\lambda}\mathrm{e}^{z/2}\tilde{O}(x^{-1}) \to \infty,\\
&v_1(x;W) = \lambda^{-\alpha}x^{-g_1/\lambda}\mathrm{e}^{-z/2}\tilde{O}(x^{-1}) \to 0.
\end{aligned}
$$

Both sets u_1, u_3 and u_1, V_1 are linearly independent,

$$
\operatorname{Wr}(u_1,u_3) = 1,\ \operatorname{Wr}(u_1,v_1) = -\Gamma^{-1}(\alpha);
$$

in particular, u_1 and v_1 form a fundamental system of solutions of (8.17) for $\operatorname{Im} W \neq 0$ and $W = 0$.

Because any solution of (8.17) is square-integrable at the origin, to study asymptotics of functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$, we use the general solution (8.30) of (8.25), performing there the substitutions $a_2u_2 \to a_2u_3$ and $u_2/2\mu \to -u_3$.

Taking into account that the potential vanishes as $x \to \infty$, we have $\psi_*(x)$, $\psi_*'(x) \overset{x\to\infty}{\longrightarrow} 0$. Using the Cauchy–Schwarz inequality for estimating the integral terms, we obtain that the desired asymptotic as $x \to 0$ is given by

$$
\begin{aligned}
&\psi_*(x) = a_1u_{1\mathrm{as}}(x) + a_2u_{3\mathrm{as}}(x) + O\left(x^{3/2}\ln x\right),\\
&\psi_*'(x) = a_1u_{1\mathrm{as}}'(x) + a_2u_{3\mathrm{as}}'(x) + O\left(x^{1/2}\ln x\right).
\end{aligned}
$$

Then we obtain $\Delta_{H^+}(\psi_*) = k_0(\overline{a_1}a_2 - \overline{a_2}a_1)$. Therefore, the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The requirement that Δ_{H^+} vanish results in the relation

$$
a_1\cos\vartheta = a_2\sin\vartheta,\ \vartheta \in \mathbb{S}(-\pi/2,\pi/2).
$$

Thus, there exists a family of s.a. Hamiltonians $\hat{H}_{3,\vartheta}$ with the domains $D_{H_{3,\vartheta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\begin{aligned}
&\psi = C\psi_{3,\vartheta\,\mathrm{as}}(x) + O(x^{3/2}\ln x),\ \psi' = C\psi'_{3,\vartheta\,\mathrm{as}}(x) + O(x^{1/2}\ln x),\\
&\psi_{3,\vartheta\,\mathrm{as}}(x) = u_{1\mathrm{as}}(x)\sin\vartheta + u_{3\mathrm{as}}(x)\cos\vartheta.
\end{aligned} \tag{8.40}$$

Therefore,

$$D_{H_{3,\vartheta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ obey } (8.40)\right\}.$$

Imposing s.a. boundary condition (8.40) on the functions (8.26) (with $a_1 = 0$), and using asymptotics (8.39), we obtain the Green's functions of the operators $\hat{H}_{3,\vartheta}$:

$$\begin{aligned}
G(x, y; W) = {}& \Omega^{-1}(W)u_{3,\vartheta}(x; W)u_{3,\vartheta}(y; W)\\
&+ \begin{cases} \tilde{u}_{3,\vartheta}(x; W)u_{3,\vartheta}(y; W),\ x > y,\\ u_{3,\vartheta}(x; W)\tilde{u}_{3,\vartheta}(y; W),\ x < y, \end{cases}
\end{aligned}$$

where

$$\begin{aligned}
\Omega(W) &= (\omega_0\cos\vartheta + \sin\vartheta)(\omega_0\sin\vartheta - \cos\vartheta)^{-1},\\
u_{3,\vartheta}(x; W) &= u_1(x; W)\sin\vartheta + u_3(x; W)\cos\vartheta,\\
\tilde{u}_{3,\vartheta}(x; W) &= u_1(x; W)\cos\vartheta - u_3(x; W)\sin\vartheta,\\
\Gamma(\alpha)\upsilon_1 &= (\omega_0\sin\vartheta - \cos\vartheta)u_{3,\vartheta} + (\omega_0\cos\vartheta + \sin\vartheta)\tilde{u}_{3,\vartheta}.
\end{aligned}$$

We note that $u_{3,\vartheta}$ and $\tilde{u}_{3,\vartheta}$ are solutions of (8.17) real entire in W, the solution $u_{3,\vartheta}$ satisfies the boundary condition (8.40), and the second summand in $G(x, y; W)$ is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty u_{2,\vartheta}(x; W)\xi(x)\mathrm{d}x,\ \xi \in D_r(\mathbb{R}_+) \cap D_{H_{3,\vartheta}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{3,\vartheta}$ ($\tilde{U} = \tilde{u}_{3,\vartheta}$), and therefore, the spectra of $\hat{H}_{3,\vartheta}$ are simple.

The derivative of the spectral function is given by $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E + i0)$.

We first consider the case $\vartheta = \pi/2$, where we have

$$u_{3,\pi/2}(x; W) = u_1(x; W),\ \ \Omega(W) = -\left[\psi(\alpha) + \ln(\lambda/k_0)\right]^{-1}.$$

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we obtain

$$\sigma'(E) = \frac{1}{2}\left(1 - \tan h\frac{\pi g_1}{2p}\right) \geq 0.$$

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 > 0$, the function $\Omega(E)$ is of the form

$$\Omega(E) = -\left[\psi(1/2 + g_1/2\tau) + \ln(2\tau/k_0)\right]^{-1},$$

which implies that for $g_1 > 0$, there is no negative part of the spectrum.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 < 0$, we have

$$\Omega(E) = -\left[\psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0)\right]^{-1},$$

which implies that there are discrete negative energy levels $\mathcal{E}_n$ in the spectrum,

$$\mathcal{E}_n = -g_1^2(1+2n)^{-2},\ \tau_n = |g_1|(1+2n)^{-1},\ n \in \mathbb{Z}_+,$$
$$\sigma'(E) = \sum_{n\in\mathbb{Z}_+} Q_n^2\delta(E - \mathcal{E}_n),\ Q_n = 2|g_1|\,(1+2n)^{-3/2}.$$

It is easy to see that for the case of $\vartheta = -\pi/2$, we obtain the same results for spectrum and eigenfunctions, as must be the case.

We thus obtain that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\pm\pi/2}$ is simple, given by spec $\hat{H}_{3,\pm\pi/2} = \mathbb{R}_+$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its generalized eigenfunctions is

$$U_E(x) = \sqrt{\sigma'(E)}u_1(x;E),\ E \geq 0.$$

For $g_1 < 0$, the spectrum of $\hat{H}_{3,\pm\pi/2}$ is simple and given by spec $\hat{H}_{3,\pm\pi/2} = \mathbb{R}_+ \cup \{\mathcal{E}_n,\ n \in \mathbb{Z}_+\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions reads

$$U_E(x) = \sqrt{\sigma'(E)}u_1(x;E),\ E \geq 0,$$
$$U_n(x) = 2|g_1|\,(1+2n)^{-3/2}\,u_1(x;\mathcal{E}_n),\ \mathcal{E}_n < 0.$$

We note that the spectrum and eigenfunctions for $\hat{H}_{3,\pi/2}$ coincide with those for $\hat{H}_1$ with $g_2 \geq 3/4$, if we set $\mu = 0$ in the respective formulas in Sect. 8.3.1.

We now turn to the case $|\vartheta| < \pi/2$. In this case, $\sigma'(E)$ can be represented as

$$\sigma'(E) = (\pi\cos^2\vartheta)^{-1}\,\mathrm{Im}\,[\omega_3(E + i0)]^{-1},$$
$$\omega_3(W) = \psi(\alpha) + \ln(\lambda/k_0) - 2\psi(1) - \tan\vartheta.$$

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, and $g_1 < 0$, we have

$$\sigma'(E) = \frac{B(E)}{\pi\cos^2\vartheta[A^2(E) + B^2(E)]}, \tag{8.41}$$

where $\omega_3(E) = A(E) - iB(E)$. The function $B(E)$ can be explicitly calculated:

$$B(E) = \frac{\pi}{2}\left(1 - \tan h\frac{\pi g_1}{2\sqrt{E}}\right) > 0,\ \forall E \geq 0, \tag{8.42}$$

whence it follows that for all $E \geq 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is purely continuous.

For $E = p^2 > 0$, $p > 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, and $g_1 > 0$, the spectral function is given by the same (8.41) and (8.42). But in this case, $B(0) = 0$ and the limit $\lim_{W\to 0}\omega_3(W)$ must be carefully examined.

At small W, we have

$$\omega_3(W) = (\tan\vartheta_{(-)} - \tan\vartheta) - \left(6g_1^2\right)^{-1} W + O(W^2),\ \tan\vartheta_{(-)} = \ln(g_1/k_0) - 2\psi(1).$$

For $\vartheta \neq \vartheta_{(-)}$, the function $\sigma'(E)$ is finite at $E = 0$. But for $\vartheta = \vartheta_{(-)}$ and small E, we have

$$\sigma'(E) = -\frac{6g_1^2}{\pi\cos^2\vartheta_{(-)}}\,\mathrm{Im}\,(E + i0)^{-1} + O(1) = \frac{6g_1^2}{\cos^2\vartheta_{(-)}}\delta(E) + O(1),$$

which means that the spectrum of the Hamiltonian $\hat{H}_{3,\vartheta_{(-)}}$ contains an eigenvalue $E = 0$.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\omega_3(E)$ is real. Therefore, $\sigma'(E)$ can differ from zero only at zero points $E_n(\vartheta)$ of $\omega_3(E)$, which yields

$$\sigma'(E) = \sum_n \left[-k_0\omega_3'(E_n(\vartheta))\cos^2\vartheta\right]^{-1}\delta(E - E_n(\vartheta)),$$
$$\omega_3(E_n(\vartheta)) = 0,\ \omega_3'(E_n(\vartheta)) < 0,$$

and

$$\partial_\vartheta E_n(\vartheta) = \left[\cos^2\vartheta\,\omega_3'(E_n(\vartheta))\right]^{-1} < 0. \tag{8.43}$$

For $g_1 > 0$, we have

$$\omega_3(E) = \psi(1/2 + g_1/2\tau) + \ln(2\tau/g_1) + \tan\vartheta_{(-)} - \tan\vartheta,$$
$$\omega_3(E) = (1/2)\ln|E| - \tan\vartheta + O(1),\quad E \to -\infty,$$
$$\omega_3(0) = \tan\vartheta_{(-)} - \tan\vartheta.$$

For $\vartheta < \vartheta_{(-)}$, the equation $\omega_3(E) = 0$ has no solution, whereas for $\vartheta \geq \vartheta_{(-)}$, it has only one solution, $E^{(-)}(\vartheta)$. Because (8.43) holds for $\partial_\vartheta E^{(-)}(\vartheta)$, $E^{(-)}(\vartheta)$ increases from $-\infty$ to 0 as ϑ changes from $\pi/2 - 0$ to $\vartheta_{(-)}$.

For $g_1 < 0$, we have

$$\omega_3(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0) - 2\psi(1) - \tan\vartheta,$$
$$\omega_3(E) = (1/2)\ln|E| - \tan\vartheta + O(1),\ E \to -\infty.$$

It is easy to verify that the equation $\omega_3(E) = 0$ has an infinite number of solutions E_n, $n \in \mathbb{Z}_+$, bounded from below and asymptotically coinciding with (8.29) as $n \to \infty$, $E_n = -g_1^2/4n^2 + O(n^{-3})$.

We thus obtain that for $g_1 > 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and given by spec $\hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \left\{E^{(-)}(\vartheta)\right\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions reads

$$\begin{aligned} U_E(x) &= \sqrt{\sigma'(E)}u_{3,\vartheta}(x;E),\ E \geq 0, \\ U(x) &= \left[-k_0 \cos^2\vartheta\,\omega_3'(E^{(-)}(\vartheta))\right]^{-1/2} u_{3,\vartheta}(x;E^{(-)}(\vartheta)) \end{aligned}$$

(the eigenvalue $E^{(-)}(\vartheta)$ exists, and therefore $E^{(-)}(\vartheta)$ and the corresponding eigenfunction $U(x)$ enter the inversion formulas only if $\vartheta \geq \vartheta_{(-)}$); for $g_1 < 0$, the spectrum of $\hat{H}_{3,\vartheta}$ is simple and given by spec $\hat{H}_{3,\vartheta} = \mathbb{R}_+ \cup \{E_n(\vartheta)\}$, and a complete orthonormalized system in $L^2(\mathbb{R}_+)$ of its (generalized) eigenfunctions reads

$$\begin{aligned} U_E(x) &= \sqrt{\sigma'(E)}u_{3,\vartheta}(x;E),\ E \geq 0, \\ U_n(x) &= \left[-k_0 \cos^2\vartheta\,\omega_3'(E_n(\vartheta))\right]^{-1/2} u_{3,\vartheta}(x;E_n(\vartheta)),\ E_n(\vartheta) < 0. \end{aligned}$$

It is possible to describe the discrete spectrum for $|\vartheta| < \pi/2$ and $g_1 < 0$ in greater detail. To this end, we represent the equation $\omega_3(E(\vartheta)) = 0$ in the equivalent form

$$f(E) = \tan\vartheta,\ f(E) = \psi(1/2 - |g_1|/2\tau) + \ln(2\tau/k_0) - 2\psi(1).$$

Then we have

$$f(-\infty) = \infty,\ \ f(\mathcal{E}_n \pm 0) = \pm\infty,\ n \in \mathbb{Z}_+.$$

Because (8.43) holds, we can see that in each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n \in \{-1\} \cup \mathbb{Z}_+$, there is one discrete eigenvalue $E_n(\vartheta)$, and $E_n(\vartheta)$ increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ϑ changes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $\mathcal{E}_{-1} = -\infty$). We note the relations

$$\lim_{\vartheta \to -\pi/2} E_{n-1}(\vartheta) = \lim_{\vartheta \to \pi/2} E_n(\vartheta) = \mathcal{E}_n.$$

8.3.4 Range 4

In this range, we have

$$g_2 < -1/4\ (\mu = i\varkappa,\ \varkappa > 0)\,.$$

Since any solution of (8.17) is square-integrable at the origin in the domain of the parameter μ under consideration, to study asymptotics of functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$, we use the general solution (8.30) of (8.25).

Since the potential is vanishing for big x, we have $\psi_*(x), \psi'_*(x) \overset{x\to\infty}{\longrightarrow} 0$; see Sect. 7.2.3. Using the Cauchy–Schwarz inequality for the estimation of integral terms, we obtain as $x \to 0$,

$$\psi_*(x) = a_1 u_{1\mathrm{as}}(x) + a_2 u_{2\mathrm{as}}(x) + O(x^{3/2}),$$

$$\psi'_*(x) = a_1 u'_{1\mathrm{as}}(x) + a_2 u'_{2\mathrm{as}}(x) + O(x^{1/2}),$$

$$u_{1\mathrm{as}}(x) = (k_0 x)^{1/2+i\varkappa},\ u_{2\mathrm{as}}(x) = (k_0 x)^{1/2-i\varkappa} = \overline{u_{1\mathrm{as}}(x)}.$$

Thus, we obtain $\Delta_{\hat{H}^+}(\psi_*) = -2i\varkappa(\overline{a_1}a_1 - \overline{a_2}a_2)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ yields $a_1 = \mathrm{e}^{2i\theta}a_2$, $\theta \in \mathbb{S}(0,\pi)$. Therefore, there exists a family of s.a. Hamiltonians $\hat{H}_{4,\theta}$ with domains $D_{H_{4,\theta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi = C\psi_{4\mathrm{as}}(x) + O(x^{3/2}),\ \psi' = C\psi'_{4\mathrm{as}}(x) + O(x^{1/2}),$$

$$\psi_{4\mathrm{as}}(x) = \mathrm{e}^{i\theta}u_{1\mathrm{as}}(x) + \mathrm{e}^{-i\theta}u_{2\mathrm{as}}(x) = \overline{\psi_{4\mathrm{as}}(x)}. \tag{8.44}$$

Therefore,

$$D_{H_{4,\theta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ obey } (8.44)\right\}.$$

Imposing s.a. boundary condition (8.44) on the functions (8.26) (with $a_1 = 0$), and using asymptotics (8.22), we obtain the Green's function of the operators $\hat{H}_{4,\theta}$,

$$G(x,y;W) = \Omega^{-1}(W)u_{4,\theta}(x;W)u_{4,\theta}(y;W)$$
$$-\frac{1}{4\varkappa k_0}\begin{cases}\tilde{u}_{4,\theta}(x;W)u_{4,\theta}(y;W),\ x > y,\\ u_{4,\theta}(x;W)\tilde{u}_{4,\theta}(y;W),\ x < y,\end{cases}$$

where

$$\Omega(W) = \frac{4i\varkappa k_0\omega_{4,\theta}(W)}{\tilde{\omega}_{4,\theta}(W)},\ \ \omega_{4,\theta}(W) = a(W) + b(W),$$

$$\tilde{\omega}_{4,\theta}(W) = a(W) - b(W),\ \ a(W) = \mathrm{e}^{i\theta}\frac{\Gamma(\beta)(\lambda/k_0)^{-i\varkappa}}{\Gamma(\alpha)},$$

$$b(W) = \mathrm{e}^{-i\theta}\frac{\Gamma(\beta_-)(\lambda/k_0)^{i\varkappa}}{\Gamma(\alpha_-)},\ \ u_{4,\theta}(x;W)$$
$$= \mathrm{e}^{i\theta}k_0^{1/2+i\varkappa}u_1(x;W) + \mathrm{e}^{-i\theta}k_0^{1/2-i\varkappa}u_2(x;W),\ \ \tilde{u}_{4,\theta}(x;W)$$
$$= i\left[\mathrm{e}^{-i\theta}k_0^{1/2-i\varkappa}u_2(x;W) - \mathrm{e}^{i\theta}k_0^{1/2+i\varkappa}u_1(x;W)\right],\ \ 4\varkappa V_1(x;W)$$
$$= -(\lambda/k_0)^{i\varkappa}k_0^{-1/2+i\varkappa}\left[i\tilde{\omega}_{4,\theta}(W)u_{4,\theta}(x;W) + \omega_{4,\theta}(W)V_\theta(x;W)\right],$$

where $u_{4,\theta}$ and $\tilde{u}_{4,\theta}$ solutions of (8.17) are real entire in W, the solution $u_{4,\theta}$ satisfies boundary conditions (8.44), and the second term in $G(x, y; W)$ is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty u_{4,\theta}(x; W)\xi(x)\mathrm{d}x,\ \xi \in D_r(\mathbb{R}_+) \cap D_{H_{4,\theta}}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{4,\theta}$ ($\tilde{U} = \tilde{u}_{4,\theta}$), and therefore, the spectra of $\hat{H}_{4,\theta}$ are simple.

The derivative of the spectral function has the form $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, $g_1 < 0$, we obtain

$$\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E) = \frac{(4\pi\varkappa k_0)^{-1}\left(1 - |D(E)|^2\right)}{(1 + D(E))(1 + \overline{D}(E))},$$

$$D(E) = \frac{a(E)}{b(E)} = \frac{\mathrm{e}^{-2i\theta}\Gamma(\beta)\Gamma(\alpha_-)\mathrm{e}^{2i\varkappa\ln(k_0/2p)}\mathrm{e}^{-\pi\varkappa}}{\Gamma(\beta_-)\Gamma(\alpha)}. \tag{8.45}$$

Because

$$|D(E)|^2 = \frac{1 + \mathrm{e}^{-2\pi\varkappa}\mathrm{e}^{-\pi g_1/p}}{1 + \mathrm{e}^{2\pi\varkappa}\mathrm{e}^{-\pi g_1/p}} < 1,\ \ p \geq 0, \tag{8.46}$$

we have spec $\hat{H}_{4,\theta} = \mathbb{R}_+$.

For $E = p^2 > 0$, $p > 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, $g_1 > 0$, expressions (8.45) and (8.46) for $\sigma'(E)$ hold.

But in this case, we have $|D(0)| = 1$ and must carefully examine the limit $\lim_{W\to 0}\Omega^{-1}(W)$.

It is easy to see that for small W, we have the representation

$$\Omega^{-1}(W) = -\frac{i}{4\varkappa k_0}\frac{1 + \mathrm{e}^{2i(\theta_0 - \theta)}}{[1 - \mathrm{e}^{2i(\theta_0-\theta)}] + iW/A} + O(1),\ A = \frac{3{g_1}^2}{\varkappa(1 + 4\varkappa^2)},$$

$$\theta_0 = \varphi - \pi[\varphi/\pi],\ \varphi = \varkappa\ln(g_1/k_0) - \theta_\Gamma + \pi/2,\ \theta_\Gamma = \frac{1}{2i}\ln\frac{\Gamma(\beta)}{\Gamma(\beta_-)},$$

where $[\varphi/\pi]$ is the entire part of φ/π. For $\theta \neq \theta_0$, the function $\sigma'(E)$ is finite at $E = 0$. But for $\theta = \theta_0$, we obtain

$$\sigma'(E + 0) = -\pi^{-1}\,(A/2\varkappa k_0)\,\mathrm{Im}\,(E + i0)^{-1} + O(1) = (A/2\varkappa k_0)\,\delta(E) + O(1),$$

which means that the spectrum of the Hamiltonian $\hat{H}_{4,\theta_0}$ with $g_1 > 0$ contains the eigenvalue $E = 0$.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\Omega(E)$ can be represented as

$$\Omega(E) = [\pi\tan\Theta(E)]^{-1},\ \Theta(E) = \theta + \theta_\Gamma - \theta_\Gamma(E) + \varkappa\ln(k_0/2\tau),$$

where

$$\theta_\Gamma(E) = \frac{1}{2i}\left[\ln\Gamma(1/2 + g_1/2\tau + i\varkappa) - \ln\Gamma(1/2 + g_1/2\tau - i\varkappa)\right]$$
$$= \begin{cases} \left.\begin{cases} -\pi|g_1|/2\tau + \varkappa\ln(|g_1|/2\tau) + O(1),\ g_1 < 0, \\ \varkappa\ln(g_1/2\tau) + O(\tau),\ g_1 > 0, \end{cases}\right\} & E \to 0, \\ \theta_\Gamma(-\infty) = \frac{1}{2i}\ln\frac{\Gamma(1/2+i\varkappa)}{\Gamma(1/2-i\varkappa)} + O(1/\tau), & E \to -\infty. \end{cases}$$

The asymptotic behavior of $\Theta(E)$ at the origin and at minus infinity is given by

$$\Theta(E) = \begin{cases} \left.\begin{cases} \pi|g_1|/2\tau + O(1),\ g_1 < 0, \\ \theta + \theta_\Gamma + \varkappa\ln(k_0/g_1) + O(\tau),\ g_1 > 0, \end{cases}\right\} & E \to 0, \\ \theta + \theta_\Gamma - \theta_\Gamma(-\infty) + \varkappa\ln(k_0/2\tau) + O(1/\tau), & E \to -\infty. \end{cases}$$

Because $\Omega(E)$ is a real function for $E < 0$, $\sigma'(E)$ can differ from zero only at the points $E_n(\theta)$ where $\Theta(E_n(\theta)) = \pi/2 + \pi n$, $n \in \mathbb{Z}$, which yields

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\theta)),\ Q_n = \left[4\varkappa k_0\Theta'(E_n(\theta))\right]^{-1/2},$$
$$\Theta'(E_n(\theta)) > 0.$$

We can obtain additional information about the discrete spectrum of $\hat{H}_{4,\theta}$. Representing the equation $\Theta(E_n(\theta)) = \pi/2 + \pi n$, $n \in \mathbb{Z}$, in the equivalent form

$$f(E_n(\theta)) = \pi/2 + \pi(n - \theta/\pi),\ f(E) = \theta_\Gamma - \theta_\Gamma(E) + \varkappa\ln(k_0/2\tau),$$
$$\partial_\theta E_n(\theta) = -\left[f'(E_n(\theta))\right]^{-1} = -\left[\Theta'(E_n(\theta))\right]^{-1} < 0,$$

we can see that the following assertions hold.

(a) The eigenvalue $E_n(\theta)$ with fixed n decreases monotonically from $E_n(0)$ to $E_n(\pi) - 0$ as θ changes from 0 to $\pi - 0$. In particular, we have $E_{n-1}(\theta) < E_n(\theta)$, $\forall n$.
(b) For any g_1, the spectrum is unbounded from below: $E_n(\theta) \to -\infty$ as $n \to -\infty$.
(c) For any θ, the negative part of the spectrum is of the form $E_n(\theta) = -k_0^2 m^2 e^{2\pi|n|/\varkappa}(1 + O(1/n))$ as $n \to -\infty$, where $m = m(g_1, g_2, \theta)$ is a scale factor, and asymptotically (as $n \to -\infty$) coincides with the negative part of the spectrum in the Calogero model with coupling constant g_2 under an appropriate identification of scale factors.
(d) For $g_1 < 0$, the discrete part of the spectrum has an accumulation point $E = 0$. More specifically, the spectrum is of the form $E_n(\theta) = -g_1^2/4n^2 + O(1/n^3)$ as $n \to \infty$ (as in all the previous ranges of the parameter g_2) and asymptotically coincides with the spectrum for $g_2 = 0$; see below.

(e) For $g_1 > 0$, the discrete spectrum has no finite accumulation points. In particular, possible values of n are restricted from above, $n \leq n_{\max}$, where

$$n_{\max} = \begin{cases} n_0 \text{ if } \begin{Bmatrix} f(0)/\pi - 1/2 = n_0, \ 0 \leq \theta < \pi \\ f(0)/\pi - 1/2 > n_0, \ 0 \leq \theta < \theta_0 \end{Bmatrix}, \\ n_0 + 1 \text{ if } f(0)/\pi - 1/2 > n_0 \text{ and } \theta_0 \leq \theta < \pi, \end{cases}$$

and the level $E = 0$ is present in the spectrum for $\theta = \theta_0$ only.

The final result is as follows: the spectrum of $\hat{H}_{4,\theta}$ is simple and given by

$$\text{spec } \hat{H}_{4,\theta} = \mathbb{R}_+ \cup \{E_n \leq 0, \ -\infty < n < n_{\max}\},$$

where $n_{\max} < \infty$ for $g_1 > 0$ and $n_{\max} = \infty$ for $g_1 < 0$, and the set of the corresponding (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}u_{4,\theta}(x; E), \ E \geq 0,$$
$$U_n(x) = Q_n u_{4,\theta}(x; E_n(\theta)), \ E_n(\theta) \leq 0,$$

forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

8.3.5 Range 5

In this range, we have

$$g_2 = 0 \ (\mu = 1/2).$$

Here, the function u_2 is not defined for $\mu = 1/2$, and we therefore use the following solutions of (8.17):

$$u_1(x; W) = x e^{-z/2} \Phi(\alpha_{1/2}, 2; z), \ u_5(x; W) = \tilde{u}_5(x; W) - g_1 \ln k_0 u_1(x; W),$$
$$v_1(x; W) = x e^{-z/2} \Psi(\alpha_{1/2}, 2; z) = \Gamma^{-1}(\alpha_{1/2}) \left[\omega_{1/2}(W) u_1(x; W) + u_5(x; W)\right],$$

where

$$\alpha_{1/2} = 1 + g_1/\lambda,$$
$$\tilde{u}_5(x; W) = e^{-z/2} x^{1/2} \left[x^{-\mu} \Phi(\alpha_-, \beta_-; z) + g_1 \Gamma(\beta_-) x^{\mu} \Phi(\alpha_+, \beta_+; z)\right]_{\mu \to 1/2},$$
$$\omega_{1/2}(W) = g_1 \mathbf{C} + g_1 \left[\psi(\alpha_{1/2}) + \ln(\lambda/k_0)\right] - g_1 - \lambda/2,$$

Here $\mathbf{C}$ is Euler's constant. The asymptotics of these functions at the origin and at infinity are respectively as follows.

As $x \to 0$, $z = \lambda x \to 0$, we have

$$u_1(x;W) = k_0^{-1} u_{1\mathrm{as}}(x) + O(x^2),\; u_5(x;W) = u_{5\mathrm{as}}(x) + O(x^2 \ln x),$$
$$\upsilon_1(x;W) = \Gamma^{-1}(\alpha_{1/2}) \left[k_0^{-1}\omega_{1/2}(W) u_{1\mathrm{as}}(x) + u_{5\mathrm{as}}(x)\right] + O(x^2 \ln x),$$
$$u_{1\mathrm{as}}(x) = k_0 x,\; u_{5\mathrm{as}}(x) = 1 + g_1 x \ln(k_0 x) + \mathbf{C} g_1 x. \tag{8.47}$$

As $x \to \infty$, $\operatorname{Im} W > 0$, we have

$$u_1(x;W) = \Gamma^{-1}(\alpha_{1/2})\lambda^{-1+g_1/\lambda} x^{+g_1/\lambda} \mathrm{e}^{z/2} \tilde{O}(x^{-1}) \to \infty,$$
$$\upsilon_1(x;W) = \lambda^{-g_1/\lambda} x^{-g_1/\lambda} \mathrm{e}^{-z/2} \tilde{O}(x^{-1}) \to 0.$$

The functions $u_1\,(x;W)$ and $u_5\,(x;W)$ are real entire in W. These functions form a fundamental system of solutions of (8.17), and the same holds for the functions u_1, υ_1 for $\operatorname{Im} W \neq 0$,

$$\mathrm{Wr}\,(u_1, u_5) = -1,\; \mathrm{Wr}\,(u_1, \upsilon_1) = -1/\Gamma(\alpha_{1/2}) = -\omega(W).$$

As we already know, for $g_2 < -1/4$, the deficiency indices of the initial symmetric operator $\hat{H}$ are $m_\pm = 1$, and therefore there exists a one-parameter family of its s.a. extensions.

For evaluating the asymmetry form Δ_{H+}, we determine the asymptotics of functions ψ_* belonging to $D^*_{\check{H}}(\mathbb{R}_+)$ at the origin using representation (8.30) of the general solution of (8.25) with $W = 0$, where the natural substitutions $a_2 u_2 \to a_2 u_5$ and $u_2/2\mu \to u_5$ must be made, and estimating the integral terms by means of the Cauchy–Schwarz inequality, which yields

$$\psi_*(x) = a_1 u_{1\mathrm{as}}(x) + a_2 u_{5\mathrm{as}}(x) + O(x^{3/2}),$$
$$\psi'_*(x) = a_1 u'_{1\mathrm{as}}(x) + a_2 u'_{5\mathrm{as}}(x) + O(x^{1/2}),$$

and we obtain $\Delta_{H+}(\psi_*) = -k_0(\overline{a_1} a_2 - \overline{a_2} a_1)$. This structure of Δ_{H+} confirms that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The requirement that Δ_{H+} vanish results in the relation $a_1 \cos\epsilon = a_2 \sin\epsilon$, $\epsilon \in \mathbb{S}\,(-\pi/2, \pi/2)$.

The final result is that for $g_2 = 0$, there exists a family of s.a. Hamiltonians $\hat{H}_{5,\epsilon}$ with domains $D_{H_{5,\epsilon}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi = C\psi_{5,\epsilon\mathrm{as}}(x) + O(x^{3/2}),\; \psi' = C\psi'_{5,\epsilon\mathrm{as}}(x) + O(x^{1/2}),$$
$$\psi_{5,\epsilon\mathrm{as}}(x) = u_{1\mathrm{as}}(k_0 x)\sin\epsilon + u_{5\mathrm{as}}(x)\cos\epsilon. \tag{8.48}$$

Therefore,

$$D_{H_{5,\epsilon}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\; \psi \text{ satisfy (8.48)}\right\}.$$

To obtain the Green's function $G(x, y; W)$ for $\hat{H}_{5,\epsilon}$, we use representation (8.26) with $a_1 = 0$ for $\psi_*(x)$ belonging to $D_{H_{4,\theta}} \subset D^*_{\check{H}}(\mathbb{R}_+)$, boundary conditions (8.48), and asymptotics (8.47). Then we obtain

$$G(x, y; W) = \Omega^{-1}(W)u_{5,\epsilon}(x; W)u_{5,\epsilon}(y; W)$$
$$-\frac{1}{k_0}\begin{cases} \tilde{u}_{5,\epsilon}(x; W)u_{5,\epsilon}(y; W), & x > y, \\ u_{5,\epsilon}(x; W)\tilde{u}_{5,\epsilon}(y; W), & x < y, \end{cases}$$

where

$$\Omega(W) = k_0\left[k_0 \sin\epsilon - \omega_{1/2}(W)\cos\epsilon\right]\left[\omega_{1/2}(W)\sin\epsilon + k_0\cos\epsilon\right]^{-1},$$
$$u_{5,\epsilon}(x; W) = k_0 u_1(x; W)\sin\epsilon + u_5(x; W)\cos\epsilon,$$
$$\tilde{u}_{5,\epsilon}(x; W) = k_0 u_1(x; W)\cos\epsilon - u_5(x; W)\sin\epsilon,$$
$$k_0\Gamma(\alpha_{1/2})\upsilon_1(x; W) = \left[\omega_{1/2}(W)\cos\epsilon - k_0\sin\epsilon\right]\tilde{u}_{5,\epsilon}(x; W)$$
$$+\left[\omega_{1/2}(W)\sin\epsilon + k_0\cos\epsilon\right]u_{5,\epsilon}(x; W).$$

We note that $u_{5,\epsilon}(x; W)$ and $\tilde{u}_{5,\epsilon}(x; W)$ are solutions of (8.17) real entire in W, the solution $u_{5,\epsilon}(x; W)$ satisfies boundary conditions (8.48), and the second summand in $G(x, y; W)$ is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty u_{5,\epsilon}(x; W)\xi(x)\mathrm{d}x,\ \xi \in D_r(\mathbb{R}_+) \cap D_{H_{5,\epsilon}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{5,\epsilon}$ ($\tilde{U} = \tilde{u}_{5,\epsilon}$), and therefore, the spectra of $\hat{H}_{5,\epsilon}$ are simple.

The derivative of the spectral function is given by $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E+i0)$.

We first consider the case of $\epsilon = \pi/2$, where we have $u_{5,\pi/2}(x; W) = k_0 u_1(x; W)$ and

$$\sigma'(E) = \left(\pi k_0^2\right)^{-1}\mathrm{Im}\,\Theta(E + i0),$$
$$\Theta(W) = g_1\psi(\alpha_{1/2}) + g_1\ln(\lambda/k_0) - \lambda/2.$$

For $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we have

$$\sigma'(E) = \frac{|g_1|\mathrm{e}^{-\pi g_1/2p}}{2k_0^2 \sin h(\pi|g_1|/2p)} \geq 0.$$

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 > 0$, $\alpha_{1/2} = 1 + g_1/2\tau$, the function $\Theta(E)$ is finite and real, whence it follows that there are no negative spectrum points.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, and $g_1 < 0$, $\alpha_{1/2} = 1 - |g_1|/2\tau$, we have

$$\sigma'(E) = \sum_{n \in \mathbb{Z}_+} \frac{4}{k_0^2} \left(\frac{|g_1|}{2+2n} \right)^3 \delta(E - \mathcal{E}_n),$$

$$\mathcal{E}_n = -\frac{g_1^2}{(2+2n)^2},\ n \in \mathbb{Z}_+ \,.$$

It is easy to see that for the case of $\epsilon = -\pi/2$, we obtain the same results for spectrum and eigenfunctions, as must be the case.

We thus obtain that for $g_1 > 0$, the spectrum of $\hat{H}_{5,\pi/2}$ is simple and given by spec $\hat{H}_{5,\pm\pi/2} = \mathbb{R}_+$. The set of generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)} u_{5,\pi/2}(x; E)$, $E \geq 0$, forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $g_1 < 0$, the spectrum of $\hat{H}_{5,\pm\pi/2}$ is simple and given by spec $\hat{H}_{5,\pm\pi/2} = \mathbb{R}_+ \cup \{\mathcal{E}_n,\ n \in \mathbb{Z}_+\}$, and the set of (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} u_{5,\pi/2}(x; E),\ E \geq 0,$$

$$U_n(x) = \frac{2}{k_0} \left(\frac{|g_1|}{2+2n} \right)^{3/2} u_{5,\pi/2}(x; \mathcal{E}_n),\ n \in \mathbb{Z}_+,$$

forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

We now turn to the case $|\epsilon| < \pi/2$, where we have

$$\sigma'(E) = \left(\pi \cos^2 \epsilon\right)^{-1} \operatorname{Im} \tilde{\Omega}^{-1}(E + i0),\ \ \tilde{\Omega}(W) = k_0 \tan \epsilon - \omega_{1/2}(W) \,.$$

For $g_1 < 0$, $E = p^2 \geq 0$, $p \geq 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, we obtain that

$$\sigma'(E) = \frac{B(E)}{\pi \cos^2 \epsilon [A^2(E) + B^2(E)]}, \tag{8.49}$$

where $\tilde{\Omega}(E) = A(E) - iB(E)$. The function $B(E)$ is explicitly given by

$$B(E) = \frac{\pi}{2} \frac{|g_1| \mathrm{e}^{-\pi g_1/2p}}{\sin h(\pi |g_1|/2p)} > 0,\ \forall p \geq 0. \tag{8.50}$$

It follows that for $g_1 < 0$, $E \geq 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is purely continuous.

For $g_1 > 0$, $E = p^2 > 0$, $p > 0$, $\lambda = 2p\mathrm{e}^{-i\pi/2}$, the derivative of the spectral function is also given by (8.49) and (8.50). But in this case, we have $B(0) = 0$, and the limit $\lim_{W \to 0} \tilde{\Omega}(W)$ has to be carefully examined. For small W, we have

$$\tilde{\Omega}(W) = (\tan \epsilon - \tan \epsilon_0) k_0 - \frac{W}{3g_1} + O(W^2),$$

$$\tan \epsilon_0 = (g_1/k_0) \left[\ln(g_1/k_0) + \mathbf{C} - 1 \right].$$

For $\epsilon \neq \epsilon_0$, the function $\sigma'(E)$ has a finite limit as $E \to 0$. But for $\epsilon = \epsilon_0$ and small E, we have

$$\sigma'(E) = \frac{3g_1}{\cos^2 \epsilon_0}\delta(E) + O(1),$$

which means that the spectrum of the Hamiltonian $\hat{H}_{5,\epsilon_0}$ has an eigenvalue $E = 0$.

For $E = -\tau^2 < 0$, $\tau > 0$, $\lambda = 2\tau$, the function $\tilde{\Omega}(E)$ is real. Therefore, $\sigma'(E)$ can differ from zero only at zero points $E_n(\epsilon)$ of $\tilde{\Omega}(E)$, and $\sigma'(E)$ is represented as

$$\sigma'(E) = \sum_n \left[-\tilde{\Omega}'(E_n(\epsilon))\right]^{-1} \delta(E - E_n(\epsilon)),$$
$$\tilde{\Omega}(E_n(\epsilon)) = 0,\ \tilde{\Omega}'(E_n(\epsilon)) < 0.$$

For $g_1 > 0$, we have

$$\tilde{\Omega}(E) = -g_1\psi(1 + g_1/2\tau) - g_1 \ln(2\tau/g_1) + \tau + k_0(\tan\epsilon - \tan\epsilon_0),$$
$$\tilde{\Omega}(E) = \sqrt{|E|} - (g_1/2)\ln|E| + O(1),\quad E \to -\infty,$$
$$\tilde{\Omega}(0) = k_0(\tan\epsilon - \tan\epsilon_0).$$

For $\epsilon > \epsilon_0$, the equation $\tilde{\Omega}(E) = 0$ has no solution, while for $\epsilon \in (-\pi/2, \epsilon_0]$ it has a unique solution $E^{(-)}(\epsilon)$. It is easy to see that

$$\partial_\epsilon E^{(-)}(\epsilon) = -k_0\left[\tilde{\Omega}'\left(E^{(-)}(\epsilon)\right)\cos^2\epsilon\right]^{-1} > 0,$$

so that $E^{(-)}(\epsilon)$ increases monotonically from $-\infty$ to 0 as ϵ changes from $-\pi/2+0$ to ϵ_0.

For $g_1 < 0$, we have

$$\tilde{\Omega}(E) = |g_1|\psi(1/2 - |g_1|/2\tau) + |g_1|\ln(2\tau/k_0) + \tau - \tilde{\epsilon},$$
$$\tilde{\epsilon} = g_1\mathbf{C} - g_1 - k_0\tan\epsilon.$$

Representing the equation $\tilde{\Omega}(E_n) = 0$ in the equivalent form

$$f(E_n) = \tilde{\epsilon},\ f(E) = |g_1|\psi(1/2 - |g_1|/2\tau) + |g_1|\ln(2\tau/k_0) + \tau,$$

we can see that:

(a)

$$f(E) \overset{E\to-\infty}{\longrightarrow} \infty,\quad f(\mathcal{E}_n \pm 0) = \pm\infty,$$

so that in each region of energy $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n \in (-1) \cup \mathbb{Z}_+$, the equation $\tilde{\Omega}(E_n) = 0$ has one solution $E_n(\epsilon)$ for any fixed ϵ, $|\epsilon| < \pi/2$, and $E_n(\epsilon)$

increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ϵ changes from $-\pi/2 + 0$ to $\pi/2 - 0$ (here, by definition, $\mathcal{E}_{-1} = -\infty$).

(b) For any fixed ϵ, $E_n(\epsilon) = -g_1^2/4n^2 + O(n^{-3})$ as $n \to \infty$, asymptotically coinciding with (8.29).

(c) The point $E = 0$ is an accumulation point of the discrete spectrum for $g_1 < 0$.

Note the relation

$$\lim_{\epsilon\to\pi/2} E_{n-1}(\epsilon) = \lim_{\epsilon\to-\pi/2} E_n(\epsilon) = \mathcal{E}_n,\ n \in \mathbb{Z}_+.$$

The above results can be briefly summarized as follows. For $g_1 < 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is simple and given by

$$\operatorname{spec} \hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E_n(\epsilon) < 0,\ n \in (-1) \cup \mathbb{Z}_+\}.$$

The (generalized) eigenfunctions of $\hat{H}_{5,\epsilon}$ given by

$$U_E(x) = \sqrt{\sigma'(E)}u_{5,\epsilon}(x; E),\ E \geq 0,$$
$$U_n(x) = \left[-\tilde{\Omega}'(E_n(\epsilon))\right]^{-1/2} u_{5,\epsilon}\left(x; E_n(\epsilon)\right),\ n \in (-1) \cup \mathbb{Z}_+,$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For $g_1 > 0$, the spectrum of $\hat{H}_{5,\epsilon}$ is simple and given by spec $\hat{H}_{5,\epsilon} = \mathbb{R}_+ \cup \{E^{(-)}(\epsilon) \leq 0\}$. For $\epsilon \in (-\pi/2, \epsilon_0]$, the (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}u_{5,\epsilon}(x; E),\ E \geq 0,$$
$$U(x) = \left[-\omega_5'\left(E^{(-)}(\epsilon)\right)\right]^{-1/2} u_{5,\epsilon}\left(x; E^{(-)}(\epsilon)\right)$$

form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. For $\epsilon > \epsilon_0$, the spectrum has no negative eigenvalues.

8.4 ESP IV

In this case,

$$V(x) = g_1 x^{-2} + g_2 x^2,\ \ x \in \mathbb{R}_+, \tag{8.51}$$

and the corresponding Schrödinger equation is

$$\psi'' - (g_1 x^{-2} + g_2 x^2)\psi + W\psi = 0\,. \tag{8.52}$$

The case $g_1 = 0$ corresponds to the harmonic oscillator potential, and the case $g_2 = 0$ was considered in Sect. 7.2. Thus, here, we assume both $g_1 \neq 0$ and $g_2 \neq 0$. In this case, we call (8.51) the *generalized Calogero potential*; see [34–36].

8.4.1 Range A

In this range, we have

$$g_2 = \upsilon^4 > 0, \;\; \upsilon > 0.$$

Here we introduce a new variable ρ and new functions $\phi_\pm$, instead of x and $\psi(x)$ in (8.52),

$$\rho = (\upsilon x)^2, \; x = \sqrt{\rho}/\upsilon, \; \rho \in \mathbb{R}_+, \; \psi(x) = \mathrm{e}^{-\rho/2}\rho^{1/4\pm\mu}\phi_\pm(\rho),$$
$$\mu = \begin{cases} \frac{1}{2}\sqrt{g_1 + 1/4}, \; g_1 \geq -1/4, \\ i\varkappa, \; \varkappa = \frac{1}{2}\sqrt{|g_1| - 1/4}, \; g_1 < -1/4. \end{cases} \tag{8.53}$$

Then $\phi_\pm(\rho)$ satisfy the equations

$$\rho d_\rho^2 \phi_\pm(\rho) + (\beta_\pm - \rho) d_\rho \phi_\pm(\rho) - \alpha_\pm \phi_\pm(\rho) = 0,$$
$$\alpha_\pm = 1/2 \pm \mu - w, \; \beta_\pm = 1 \pm 2\mu, \;\; w = W/4\upsilon^2,$$

which have as solutions the confluent hypergeometric functions $\Phi(\alpha_\pm, \beta_\pm; \rho)$ and $\Psi(\alpha_\pm, \beta_\pm; \rho)$ (see [1, 20, 81]).

In what follows, we will use the following three solutions of (8.52):

$$u_1(x; W) = \mathrm{e}^{-\rho/2}\rho^{1/4+\mu}\Phi(\alpha, \beta; \rho), \; \alpha = \alpha_+, \; \beta = \beta_+,$$
$$u_2(x; W) = \mathrm{e}^{-\rho/2}\rho^{1/4-\mu}\Phi(\alpha_-, \beta_-; \rho) = u_1(x; W)|_{\mu \to -\mu},$$
$$V_1(x; W) = \mathrm{e}^{-\rho/2}\rho^{1/4+\mu}\Psi(\alpha, \beta; \rho) = \frac{\Gamma(1-\beta)}{\Gamma(\alpha_-)}u_1(x; W) + \frac{\Gamma(\beta - 1)}{\Gamma(\alpha)}u_2(x; W).$$

We note that $u_2(x; W)$ is not defined for $2\mu = m \in \mathbb{N}$. The function $V_1(x; W)$ is real entire in W for any g_1, while $u_1(x; W)$ is real entire in W for $g_1 \geq -1/4$ ($\mu \geq 0$), and $u_2(x; W)$ is real entire in W for $g_1 \geq -1/4$ and $2\mu \neq m$. If $g_1 < -1/4$ ($\mu = i\varkappa$), then $u_1(x; W)$ and $u_2(x; W)$ are entire in W and $u_2(x; E) = \overline{u_1(x; E)}$.

Below, we list some asymptotics of the introduced functions as $x \to 0$ and $x \to \infty$; see [1, 20, 81].

For $x \to \infty$ ($\rho \to \infty$), we have

$$u_1(x; W) = \Gamma^{-1}(\alpha)\Gamma(\beta)\mathrm{e}^{\rho/2}\rho^{-1/4-w}\tilde{O}(\rho^{-1})$$
$$= O(x^{-1/2-2w}\mathrm{e}^{\rho/2}) \to \infty, \;\; \alpha \notin \mathbb{R}_-,$$
$$V_1(x; W) = \mathrm{e}^{-\rho/2}\rho^{-1/4+w}\tilde{O}(\rho^{-1}) = O\left(x^{-1/2+2w}\mathrm{e}^{-\rho/2}\right) \to 0.$$

For $x \to 0$ ($\rho \to 0$), we have

$$\begin{aligned} u_1 &= \rho^{1/4+\mu}\tilde{O}(\rho) = (\upsilon x)^{1/2+2\mu}\tilde{O}(x^2) \to 0, \\ u_2 &= \rho^{1/4-\mu}\tilde{O}(\rho) = (\upsilon x)^{1/2+2\mu}\tilde{O}(x^2) \to 0, \;\; \alpha \notin \mathbb{R}_-, \end{aligned} \tag{8.54}$$

and

$$V_1(x;W) = \begin{cases} \frac{\Gamma(\beta-1)}{\Gamma(\alpha)}(\upsilon x)^{1/2-2\mu}\tilde{O}(x^2), \; g_1 > 3/4, \\ \Gamma^{-1}(\alpha)(\upsilon x)^{-1/2}\tilde{O}(x^2\ln x), \; g_1 = 3/4, \\ \frac{\Gamma(\beta-1)}{\Gamma(\alpha)}(\upsilon x)^{1/2-2\mu} + \frac{\Gamma(1-\beta)}{\Gamma(\alpha_-)}(\upsilon x)^{1/2+2\mu} \\ +O(x^{5/2-2\mu}), \; 3/4 > g_1 \neq -1/4, \\ \Gamma^{-1}(\upsilon x)^{1/2}[2\psi(1) - \psi(\alpha) - 2\ln(\upsilon x)] \\ +O(x^{5/2}\ln x), \; g_1 = -1/4. \end{cases} \tag{8.55}$$

Regarding

$$\mathrm{Wr}\,(u_1,u_2) = -4\mu\upsilon, \;\; \mathrm{Wr}\,(u_1,V_1) = -2\upsilon\Gamma(\beta)/\Gamma(\alpha) = -\omega(W),$$

solutions u_1 and V_1 are linearly independent and form a fundamental system of solutions of (8.52) for $\operatorname{Im} W \neq 0$.

We note that for $g_1 \geq 3/4$, the function $V_1(x;W)$ is not square-integrable at the origin, whereas for $g_1 < 3/4$ it is (moreover, any solution is square-integrable at the origin). This means that for $g_1 \geq 3/4$, (8.52) has no square-integrable solutions, and deficient indices of the initial symmetric operator $\hat{H}$ (with the domain $D_H = \mathcal{D}(\mathbb{R}_+)$) are zero, and $\hat{H}_1 = \hat{H}^+$ ($D_{H_1} = D^*_{\check{H}}(\mathbb{R}_+)$ is the unique s.a. extension of $\hat{H}$. For $g_1 < 3/4$ there is one square-integrable solution, $V_1(x;W)$, and the deficiency indices of $\hat{H}$ are $m_\pm = 1$.

The adjoint $\hat{H}^+$ is defined on functions ψ_* from the domain $D^*_{\check{H}}(\mathbb{R}_+)$. Such functions satisfy the equation

$$\check{H}\psi_*(x) = \eta(x) \in L^2(\mathbb{R}_+)\,. \tag{8.56}$$

The potential under consideration is bounded from below by $-(|g_2| + 1)x^2$ as $x \to \infty$. In such a case, the boundary form at infinity is zero, $[\psi_*, \psi_*](\infty) = 0$, $\forall\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$; see Sect. 7.1. The asymptotic behavior as $x \to 0$ can be found by analyzing solutions of (8.56). For $g_1 \geq 3/4$, one can represent its general solution in the following form:

$$\begin{aligned} &\psi_*(x) = c_1u_1(x;0) + c_2V_1(x;0) + I(x), \\ &I(x) = \omega^{-1}(0)\left[u_1(x;0)\int_x^\infty V_1(y;0)\eta(y)\mathrm{d}y + V_1(x;0)\int_0^x u_1(y;0)\eta(y)\mathrm{d}y\right]. \end{aligned}$$

Using the Cauchy–Schwarz inequality, we obtain that $I(x)$ is bounded as $x \to \infty$ and $I(x) \sim O(x^{3/2})$ as $x \to 0$ (with logarithmic accuracy for $g_1 = 3/4$; see below). The condition $\psi_* \in L^2(\mathbb{R}_+)$ implies $c_1 = c_2 = 0$, so that the asymptotic as $x \to 0$ is due to the term $I(x)$.

For $g_1 < 3/4$, one can represent the general solution in the form

$$\psi_*(x) = c_1 u_1(x;0) + c_2 V_1(x;0) + I_1(x),$$
$$I_1(x) = \omega^{-1}(0)\left[V_1(x;0)\int_0^x u_1(y;0)\eta(y)\mathrm{d}y - u_1(x;0)\int_0^x V_1(y;0)\eta(y)\mathrm{d}y\right].$$

Using the Cauchy–Schwarz inequality, we obtain that $I_1(x) \sim O(x^{3/2})$ as $x \to 0$ (with logarithmic accuracy for $g_1 = -1/4$; see below). Analyzing the asymptotics of $u_1(x;0)$ and $V_1(x;0)$ as $x \to 0$, we obtain

$$\psi_*(x) = \psi_{*\mathrm{as}}(x) + \begin{cases} O(x^{3/2}),\ g_1 \neq 3/4, -1/4, \\ O(x^{3/2}\sqrt{\ln x}),\ g_1 = 3/4, \\ O(x^{3/2}\ln x),\ g_1 = -1/4, \end{cases}$$
$$\psi_*'(x) = \psi_{*\mathrm{as}}'(x) + \begin{cases} O(x^{1/2}),\ g_1 \neq 3/4, -1/4, \\ O(x^{1/2}\sqrt{\ln x}),\ g_1 = 3/4, \\ O(x^{1/2}\ln x),\ g_1 = -1/4, \end{cases} \tag{8.57}$$

where

$$\psi_{*\mathrm{as}}(x) = \begin{cases} 0,\quad g_1 \geq 3/4, \\ c_1(\upsilon x)^{1/2+2\mu} + c_2(\upsilon x)^{1/2-2\mu},\quad g_1 < 3/4,\ g_1 \neq -1/4, \\ c_1(\upsilon x)^{1/2} + 2c_2(\upsilon x)^{1/2}\ln(\upsilon x),\quad g_1 = -1/4. \end{cases}$$

The general solution of the inhomogeneous equation

$$\left(\check{H} - W\right)\psi(x) = \eta(x) \in L^2(\mathbb{R}_+),\ \mathrm{Im}\, W \neq 0,$$

can be represented as

$$\psi(x) = c_1 u_1(x;W) + c_2 V_1(x;W) + I(x;W),\ I(x;W) = \omega^{-1}(W) \tag{8.58}$$
$$\times\left[u_1(x;W)\int_x^\infty V_1(y;W)\eta(y)\mathrm{d}y + V_1(x;W)\int_0^x u_1(y;W)\eta(y)\mathrm{d}y\right].$$

Estimates of the integral terms with the help of the Cauchy–Schwarz inequality show that $I(x)$ is bounded as $x \to \infty$. The condition $\psi \in L^2(\mathbb{R}_+)$ implies $c_1 = 0$.

If $g_1 \geq 3/4$, then $I(x) \sim O(x^{3/2})$ as $x \to 0$ (with logarithmic accuracy for $g_1 = 3/4$), and $V_1(x;W)$ is not square-integrable at the origin. The condition $\psi \in L^2(\mathbb{R}_+)$ implies $c_2 = 0$.

For $g_1 < 3/4$, it is convenient to use another representation for the general solution (8.58):

$$\psi(x) = c_2 V_1(x;W) + \omega^{-1}(W)u_1(x;W)\int_0^\infty V_1(y;W)\eta(y)\mathrm{d}y + I_1(x;W),$$

$$I_1(x;W) = \omega^{-1}(W)\left[V_1(x;W)\int_0^x u_1(y;W)\eta(y)\mathrm{d}y \right.$$
$$\left. -u_1(x;W)\int_0^x V_1(y;W)\eta(y)\mathrm{d}y\right]. \tag{8.59}$$

Estimates with the help of the Cauchy–Schwarz inequality give $I_1(x) \sim O(x^{3/2})$ as $X \to 0$ (with logarithmic accuracy for $g_1 = -1/4$).

8.4.1.1 Subrange $g_1 \geq 3/4$ ($\mu \geq 1/2$)

For such g_1, as was mentioned above, $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$. Its Green's function can be found from (8.58) with $c_1 = c_2 = 0$:

$$G(x,y;W) = \omega^{-1}(W)\begin{cases} V_1(x;W)u_1(y;W), \ x > y, \\ u_1(x;W)V_1(y;W), \ x < y. \end{cases} \tag{8.60}$$

The Green's function allows one to calculate the derivative of the spectral function,

$$\sigma'(E) = \pi^{-1}\,\mathrm{Im}\left[\omega^{-1}(W)\frac{V_1(c;W)}{u_1(c;W)}\right]_{W=E+i0}. \tag{8.61}$$

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x u_1(x;W)\xi(x), \ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ ($\tilde{U} = V_1$), and therefore, the spectrum of $\hat{H}_1$ is simple.

In the ranges $m - 1 < 2\mu < m + 1$, $m \geq 1$, the function $V_1(x;W)$ can be represented as

$$V_1(x;W) = A_m(W)u_1(x;W) + \frac{\omega(W)}{4\mu\upsilon}V_{(m)}(x;W),$$

$$A_m(W) = \frac{\pi}{\sin(2\pi\mu)}\left[\frac{\Gamma(\alpha_{+m})}{m!\Gamma(\alpha)\Gamma(\alpha_{-m})} - \frac{1}{\Gamma(\alpha_-)\Gamma(\beta)}\right],$$

$$V_{(m)}(x;W) = \mathrm{e}^{-\rho/2}\rho^{1/2+\mu}\Gamma(\beta_-)\left[\frac{\rho^{-2\mu}}{\Gamma(\beta_-)}\Phi(\alpha_-,\beta_-;\rho)\right.$$
$$\left. -\frac{\Gamma(\alpha_{+m})}{m!\Gamma(\alpha_{-m})}\Phi(\alpha,\beta;\rho)\right], \ \alpha_{\pm m} = 1/2 \pm m/2 - w.$$

Using the relation (8.27), one can verify that $V_{(m)}(x;W)$ is well defined for any W and for $m-1<2\mu<m+1$, and $V_{(m)}(x;E)$ is real. The same holds for $A_m(W)$. As a result, we obtain

$$\sigma'(E)=\frac{A_m(E)}{2\pi\upsilon\Gamma(\beta)}\operatorname{Im}\Gamma(\alpha)|_{W=E+i0}\,,\ \ m-1<2\mu<m+1.$$

Let $|\Gamma(\alpha)|<\infty$. Then $\Gamma(\alpha)$ is real for $W=E$. Therefore, the quantity $\operatorname{Im}\Gamma(\alpha)|_{W=E+i0}$ can differ from zero only for $\alpha=-n$, $n\in\mathbb{Z}_+$, or for the energies $E_n=2\upsilon^2(1+2n+2\mu)$. Near these points, we have

$$\operatorname{Im}\Gamma(\alpha)|_{W=E+i0}=(-1)^n\frac{4\upsilon^2\pi}{n!}\delta(E-E_n),$$

see Lemma 5.17, so that the derivative of the spectral function reads

$$\sigma'(E)=\sum_{n\in\mathbb{Z}_+}Q_n^2\delta(E-E_n),\ Q_n=\sqrt{\frac{2\upsilon\Gamma(\beta+n)}{n!\Gamma^2(\beta)}}.$$

Thus, the simple spectrum of $\hat{H}_1$ reads spec $\hat{H}_1=\{E_n,\ n\in\mathbb{Z}_+\}$, and the set of eigenfunctions $U_n(x)=Q_nu_1(x;E_n)$, $n\in\mathbb{Z}_+$ of $\hat{H}_1$ forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

8.4.1.2 Subrange $3/4>g_1>-1/4$ $(1/2>\mu>0)$

Using the asymptotics (8.57), we obtain $\Delta_{H^+}(\psi_*)=-4\mu\upsilon(\overline{c_1}c_2-\overline{c_2}c_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm=1$. At the same time, the condition $\Delta_{H^+}(\psi_*)=0$ implies $c_1\cos\nu=c_2\sin\nu$, $\nu\in\mathbb{S}(-\pi/2,\pi/2)$. Thus, in the subrange under consideration, there exists a family of s.a. $\hat{H}_{2,\nu}$ parameterized by ν with domains $D_{H_{2,\nu}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x\to 0$,

$$\begin{aligned}&\psi(x)=C\psi_{\mathrm{as}}(x)+O(x^{3/2}),\ \psi'(x)=C\psi'_{\mathrm{as}}(x)+O(x^{1/2}),\\&\psi_{\mathrm{as}}(x)=(\upsilon x)^{1/2+2\mu}\sin\nu+(\upsilon x)^{1/2-2\mu}\cos\nu.\end{aligned}\tag{8.62}$$

Therefore,

$$D_{H_{2,\nu}}=\{\psi:\psi\in D^*_{\check{H}}(\mathbb{R}_+),\ \psi\text{ satisfy (8.62)}\}.$$

Imposing the boundary conditions (8.62) on the functions (8.59) and using the asymptotics (8.54) and (8.55), we obtain the Green's function of the Hamiltonian $\hat{H}_{2,\nu}$,

$$G(x,y;W)=\Omega^{-1}(W)u_{2,\nu}(x;W)u_{2,\nu}(y;W)\\-\frac{1}{4\mu\upsilon}\begin{cases}\tilde{u}_{2,\nu}(x;W)u_{2,\nu}(y;W),\ x>y,\\u_{2,\nu}(x;W)\tilde{u}_{2,\nu}(y;W),\ x<y,\end{cases}$$

where

$$\varOmega(W) = 4\mu\upsilon[\cos\nu - f(W)\sin\nu]^{-1}(\sin\nu + f(W)\cos\nu),$$

$$f(W) = \frac{\Gamma(\alpha)\Gamma(\beta_-)}{\Gamma(\alpha_-)\Gamma(\beta)},$$

$$u_{2,\nu}(x;W) = u_1(x;W)\sin\nu + u_2(x;W)\cos\nu,$$

$$\tilde{u}_{2,\nu}(x;W) = u_1(x;W)\cos\nu - u_2(x;W)\sin\nu.$$

We note that $u_{2,\nu}(x;W)$ and $\tilde{u}_{2,\nu}(x;W)$ are solutions of (8.52) real entire in W, $u_{2,\nu}(x;W)$ satisfies the boundary condition (8.62), and the second summand in $G(x,y;W)$ is real for real $W = E$.

Consider the guiding functional

$$\varPhi(\xi;W) = \int_0^\infty \mathrm{d}x u_{2,\nu}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{2,\nu}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{2,\nu}$ ($\tilde{U} = \tilde{u}_{2,\nu}$), and therefore, the spectra of $D_{H_{2,\nu}}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\operatorname{Im}\varOmega^{-1}(E + i0)$.

The function $\varOmega^{-1}(E)$ is real for any E where $\varOmega(E) \neq 0$. That is why only the points $E_n(\nu)$ satisfying the equation $\varOmega(E_n(\nu)) = 0$ can provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\nu)),\ Q_n = \sqrt{-[4\mu\upsilon\varOmega'(E_n(\nu))]^{-1}}. \tag{8.63}$$

As a result, we find that the simple spectrum of $\hat{H}_{2\nu}$ reads spec $\hat{H}_{2\nu} = \{E_n(\nu)\}$, and the set of its eigenfunctions $U_n(x) = Q_n u_{2\nu}(x;E_n(\nu))$ forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

One can make some remarks on the spectrum structure. For $\nu = \pm\pi/2$, we have

$$\sigma'(E) = \sum_{n\in\mathbb{Z}_+} Q_n^2\delta(E - \mathcal{E}_n),\ Q_n = \sqrt{\frac{2\upsilon\Gamma(\beta+n)}{n!\Gamma^2(\beta)}},$$

$$\mathcal{E}_n = E_n(\pm\pi/2) = 2\upsilon^2(1 + 2\mu + 2n).$$

For $|\nu| < \pi/2$, the expression (8.63) for $\sigma'(E)$ can be reduced to the following form:

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\nu)),\ Q_n = \sqrt{-\left[4\mu\upsilon\omega'_{2,\nu}(E_n(\nu))\right]^{-1}},$$

$$\omega_{2,\nu}(E_n(\nu)) = 0,\ \omega_{2,\nu}(W) = f(W) + \tan\nu,\ \omega'_{2,\nu}(E_n(\nu)) < 0.$$

We note that $\omega_{2,\nu}(E_n(\nu)) = 0 \Longrightarrow f(E_n(\nu)) = -\tan\nu$ and the function $f(E)$ has the properties

$$f(E) \overset{E\to-\infty}{\longrightarrow} \infty;\ \ f(\mathcal{E}_n \pm 0) = \pm\infty,\ n \in \mathbb{Z}_+;$$
$$f(E_k(0)) = 0,\ E_k(0) = 2\upsilon^2(1 - 2\mu + 2k),\ k \in \mathbb{Z}_+;$$
$$E_n(0) < \mathcal{E}_n < E_{n+1}(0) < \mathcal{E}_{n+1},\ n \in \mathbb{Z}_+.$$

Since

$$\partial_\nu E_n(\nu) = -[f'(E_n(\nu))\cos^2\nu]^{-1} = [-\omega'_{2,\nu}(E_n(\nu))\cos^2\nu]^{-1} > 0,$$

we can see that in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, for fixed $\nu \in (-\pi/2, \pi/2)$, there is one solution $E_n(\nu)$ of $\omega_{2,\nu}(E_n(\nu)) = 0$ (we set formally $\mathcal{E}_{-1} = -\infty$); the solution $E_n(\nu)$ increases monotonically from $\mathcal{E}_{n-1} + 0$ (passing $E_n(0)$ at $\nu = 0$) to $\mathcal{E}_n - 0$ as ν changes from $-\pi/2 + 0$ to $\pi/2 - 0$. Note the relation

$$\lim_{\nu\to\pi/2} E_n(\nu) = \lim_{\nu\to-\pi/2} E_{n+1}(\nu) = \mathcal{E}_n,\ n \in \mathbb{Z}_+.$$

We stress that all the results (for spectrum, spectral function, and eigenfunctions) obtained for $3/4 > g_1 > -1/4$ $(1/2 > \mu > 0)$, $\nu = \pm\pi/2$, and $\nu = 0$ can be obtained from the case $g_1 \geq 3/4$ (setting there in addition $\mu \to -\mu$ in the case $\nu = 0$).

8.4.1.3 Subrange $g_1 = -1/4$ ($\mu = 0$)

Using the asymptotics (8.57), we obtain $\Delta_{H^+}(\psi_*) = 2\upsilon(\overline{c_1}c_2 - \overline{c_2}c_1)$, which means that deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $c_1\cos\vartheta = c_2\sin\vartheta$, $\vartheta \in \mathbb{S}(-\pi/2, \pi/2)$. Thus, in the subrange under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{3,\vartheta}$ parameterized by ϑ with domains $D_{H_{3\vartheta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{\rm as}(x) + O(x^{3/2}),\ \psi'(x) = C\psi'_{\rm as}(x) + O(x^{1/2}),$$
$$\psi_{\rm as}(x) = (\upsilon x)^{1/2}\sin\vartheta + 2(\upsilon x)^{1/2}\ln(\upsilon x)\cos\vartheta. \tag{8.64}$$

Therefore,

$$D_{H_{3\vartheta}} = \{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy } (8.64)\}.$$

Imposing the boundary conditions (8.64) on the functions (8.59), where now

$$u_1(x;W) = \rho^{1/4}\mathrm{e}^{-\rho/2}\Phi(\alpha_0, 1; \rho),\ \alpha_0 = \alpha|_{\mu=0} = 1/2 - w,\ w = W/4\upsilon^2,$$
$$V_1 = \rho^{1/4}\mathrm{e}^{-\rho/2}\Psi(\alpha_0, 1; \rho) = \Gamma^{-1}(\alpha_0)\left[(2\psi(1) - \psi(\alpha_0))\, u_1(x;W) - u_3(x;W)\right],$$
$$u_3(x;W) = \rho^{1/4}\mathrm{e}^{-\rho/2}\partial_\mu\left[\rho^\mu\Phi(1/2+\mu-w, 1+2\mu;\rho)\right]_{\mu=0},$$

using asymptotics (8.54) and (8.55), and the representation

$$\begin{aligned}
\Gamma(\alpha_0)V_1(x;W) &= -A(W)u_{3,\vartheta}(x;W) - B(W)\tilde{u}_{3,\vartheta}(x;W),\\
u_{3,\vartheta}(x;W) &= u_1(x;W)\sin\vartheta + u_3(x;W)\cos\vartheta,\\
\tilde{u}_{3,\vartheta}(x;W) &= u_1(x;W)\cos\vartheta - u_3(x;W)\sin\vartheta,\\
A(W) &= f(W)\sin\vartheta + \cos\vartheta,\ B(W) = f(W)\cos\vartheta - \sin\vartheta,\\
f(W) &= \psi(\alpha_0) - 2\psi(1),
\end{aligned}$$

we obtain the Green's function of the Hamiltonian $\hat{H}_{3\vartheta}$,

$$\begin{aligned}
G(x,y;W) &= \Omega^{-1}(W)u_{3,\vartheta}(x;W)u_{3,\vartheta}(y;W)\\
&\quad + \frac{1}{2\upsilon}\begin{cases}\tilde{u}_{3,\vartheta}(x;W)u_{3,\vartheta}(y;W), & x > y,\\ u_{3,\vartheta}(x;W)\tilde{u}_{3,\vartheta}(y;W), & x < y,\end{cases}
\end{aligned} \tag{8.65}$$

where $\Omega(W) = 2\upsilon B(W)/A(W)$.

We note that $u_{3,\vartheta}(x;W)$ and $\tilde{u}_{3,\vartheta}(x;W)$ are solutions of (8.52) that are real entire in W satisfying boundary condition (8.64), and the second term on the right-hand side of (8.65) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x u_{3,\vartheta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{3\vartheta}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{3,\vartheta}$ ($\tilde{U} = \tilde{u}_{3,\vartheta}$), and therefore, the spectra of $\hat{H}_{3\vartheta}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E + i0)$.

One can see that all finite values of the function $\Omega^{-1}(E)$ are real. That is why the only points $E_n(\vartheta)$ that satisfy the equation $\Omega(E_n(\vartheta)) = 0$ provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\vartheta)),\ Q_n = \sqrt{-(2\upsilon\Omega'(E_n(\vartheta)))^{-1}}. \tag{8.66}$$

Taking this into account, we see that the simple spectra of $\hat{H}_{3\vartheta}$ are spec $\hat{H}_{3\vartheta} = \{E_n(\vartheta)\}$ and the eigenfunctions $U_n(x) = Q_n u_{3\vartheta}(x; E_n(\vartheta))$ of $\hat{H}_{3\vartheta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

One can make some remarks about the spectrum structure. For $\vartheta = \pm\pi/2$, we have

$$\sigma'(E) = -(2\pi\upsilon)^{-1}\operatorname{Im}\psi(\alpha_0)\Big|_{W=E+i0} = \sum_{n\in\mathbb{Z}_+} 2\upsilon\delta(E-\mathcal{E}_n),$$

$$\mathcal{E}_n = E_n(\pm\pi/2) = 2\upsilon^2(1+2n).$$

For $|\vartheta| < \pi/2$, expression (8.66) can be written as

$$\sigma'(E) = \sum_n Q_n^2\delta(E-E_n(\vartheta)),\ Q_n = \sqrt{-(4\mu\upsilon f'(E_n(\vartheta)))^{-1}},$$

$$f(E_n(\vartheta)) = \tan\vartheta,\ f'(E_n(\vartheta)) < 0,$$

where

$$f(E) \overset{E\to-\infty}{\longrightarrow} \infty,\ f(E_n^{(\pm\pi/2)} \pm 0) = \pm\infty,\ n\in\mathbb{Z}_+,$$

$$\partial_\vartheta E_n(\vartheta) = [f'(E_n(\vartheta))\cos^2\vartheta]^{-1} < 0.$$

We can see that in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, for fixed $\vartheta \in (-\pi/2, \pi/2)$, there is one solution $E_n(\vartheta)$ of the equation $f(E_n(\vartheta)) = \tan\vartheta$ (we set formally $\mathcal{E}_{-1} = \infty$); the solution $E_n(\vartheta)$ increases monotonically from $\mathcal{E}_{n-1}+0$ to $\mathcal{E}_n - 0$ as ϑ changes from $\pi/2 - 0$ to $-\pi/2 + 0$. Note the relation

$$\lim_{\vartheta\to-\pi/2} E_n(\vartheta) = \lim_{\vartheta\to\pi/2} E_{n+1}(\vartheta) = \mathcal{E}_n,\ n\in\mathbb{Z}_+.$$

We stress that all the results (spectrum and eigenfunction) for $g_1 = -1/4$ $(\mu = 0)$, $\vartheta = \pm\pi/2$, can be obtained from the case $g_1 \geq 3/4$ by a formal limit $\mu \to 0$.

8.4.1.4 Subrange $g_1 < -1/4$ ($\mu = i\varkappa$, $\varkappa > 0$)

Using the asymptotics (8.57), we obtain $\Delta_{H+}(\psi_*) = -4i\varkappa\upsilon(\overline{c_1}c_2 - \overline{c_2}c_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H+}(\psi_*) = 0$ implies $c_1 = \mathrm{e}^{2i\theta}c_2$, $\theta \in \mathbb{S}(0,\pi)$.

Thus, in the subrange under consideration, there exists a family of s.a. Hamiltonians parameterized by θ with domains $D_{H_{4\theta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{\text{as}}(x) + O(x^{3/2}),\ \psi'(x) = C\psi'_{\text{as}}(x) + O(x^{1/2}),$$

$$\psi_{\text{as}}(x) = \mathrm{e}^{i\theta}(\upsilon x)^{1/2+2i\varkappa} + \mathrm{e}^{-i\theta}(\upsilon x)^{1/2-2i\varkappa}. \tag{8.67}$$

Therefore,

$$D_{H_{4\theta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy } (8.67)\right\}.$$

Imposing the boundary conditions (8.67) on the functions (8.59), using the asymptotics (8.54), (8.55), and representing the function $V_1(x; W)$ in the form

$$\begin{aligned}
V_1(x; W) &= -\frac{1}{4\varkappa}\left[A(W)u_{4,\theta}(x; W) + B(W)\tilde{u}_{4,\theta}(x; W)\right],\\
u_{4,\theta}(x; W) &= \mathrm{e}^{i\theta}u_1(x; W) + \mathrm{e}^{-i\theta}u_2(x; W),\\
\tilde{u}_{4,\theta}(x; W) &= i\,[\mathrm{e}^{-i\theta}u_2(x; W) - \mathrm{e}^{i\theta}u_1(x; W)],\\
A(W) &= i\left[\mathrm{e}^{i\theta}\omega_+(W) - \mathrm{e}^{-i\theta}\omega_-(W)\right],\\
B(W) &= \mathrm{e}^{i\theta}\omega_+(W) + \mathrm{e}^{-i\theta}\omega_-(W),\ \omega_\pm(W) = \Gamma(\beta_\pm)/\Gamma(\alpha_\pm),
\end{aligned}$$

where $u_{4,\theta}(x; W)$ and $\tilde{u}_{4,\theta}(x; W)$ are real entire solutions of (8.52) and $u_{4,\theta}(x; W)$ satisfies the boundary conditions (8.67), we obtain the Green's function of the Hamiltonian $\hat{H}_{4\theta}$,

$$\begin{aligned}
G(x, y; W) = {}& \Omega^{-1}(W)\,u_{4,\theta}(x; W)u_{4,\theta}(y; W)\\
&- \frac{1}{8\varkappa\upsilon}\begin{cases}\tilde{u}_{4,\theta}(x; W)u_{4,\theta}(y; W),\ x > y,\\ u_{4,\theta}(x; W)\tilde{u}_{4,\theta}(y; W),\ x < y,\end{cases}
\end{aligned} \tag{8.68}$$

where $\Omega(W) = -8\varkappa\upsilon B(W)/A(W)$ and the second term on the right-hand side of (8.68) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_{4,\theta}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{4\theta}}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{4,\theta}$ ($\tilde{U} = \tilde{u}_{4,\theta}$), and therefore the spectra of $\hat{H}_{4\theta}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

The function $\Omega^{-1}(E)$ is real for any values of E where $|\Omega^{-1}(E)| < \infty$. That is why only the points $E_n(\theta)$ obeying the equation $\Omega(E_n(\theta)) = 0, n \in \mathbb{Z}$, can provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\theta)),\ Q_n = \left(8\varkappa\upsilon\Omega'(E_n(\theta))\right)^{-1/2},\ \Omega'(E_n(\theta)) > 0.$$

Thus, the simple spectrum of $\hat{H}_{4\theta}$ is spec $\hat{H}_{4\theta} = \{E_n(\theta)\}$ and the eigenfunctions $U_n(x) = Q_n u_{4\theta}(x; E_n(\theta))$ of the Hamiltonian $\hat{H}_{4\theta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

One can make some remarks about the spectrum structure. Let us represent the function $\Omega^{-1}(E)$ in the following form:

$$\Omega^{-1}(E) = \frac{1}{8\varkappa\upsilon}\tan[\theta + f(E)], \quad f(E) = \theta_\Gamma - \theta_\Gamma(E),$$

$$\theta_\Gamma = \frac{1}{2i}\ln\frac{\Gamma(1+2i\varkappa)}{\Gamma(1-2i\varkappa)}, \; \theta_\Gamma(E) = \frac{1}{2i}[\ln\Gamma(1/2+z_+) - \ln\Gamma(1/2+z_-)],$$

$$z_\pm = -E/4\upsilon^2 \pm i\varkappa = |-E/4\upsilon^2 \pm i\varkappa|\mathrm{e}^{\pm i\varphi}, \; +0 \le \varphi = \operatorname{arccot}(E/\varkappa) \le \pi - 0,$$

$$f(E) = \begin{cases} -\varkappa\ln(|E|/4\upsilon^2) + O(1), \; E \to -\infty, \\ \pi E + O(1), \; E \to \infty, \end{cases}$$

so that the equation $\Omega(E_n(\theta)) = 0$ is reduced to one $f(E_n(\theta)) = \pi/2 + \pi(n - \theta/\pi)$. On the other side,

$$\partial_\theta E_n(\theta) = -\left(f'(E_n(\theta))\right)^{-1} = -\left(\Omega'(E_n(\theta))\right)^{-1} < 0.$$

This implies that the eigenvalue $E_n(\theta)$ (for a fixed θ) decreases monotonically from $E_n(0)$ to $E_n(\pi) = E_{n-1}(0)$ as θ changes from 0 to π. In particular, $E_{n-1}(\theta) < E_n(\theta)$, $\forall n$.

For any g_2, the spectrum is unbounded from below. For any θ, the negative energy levels have the asymptotic (as $n \to -\infty$) form $E_n = -m^2\mathrm{e}^{2\pi|n|/\varkappa}(1 + O(1/n))$, which tends asymptotically to the spectrum of the Calogero problem (with $\alpha = g_1$); $m = m(g_1, g_2, \theta)$ is a scale factor.

For $n \to \infty$, the spectrum has the form $E_n(\theta) = 4\upsilon^2 n + O(1)$ (this fact holds for any range of the parameter g_1). As an exercise, the reader can compare this spectrum with the harmonic oscillator spectrum.

8.4.2 Range B

In this range, we have

$$g_2 = -\upsilon^4 > 0, \; \upsilon > 0.$$

Here, we introduce a new variable $z = i\rho$ and new functions $\phi_\pm$, instead of x and $\psi(x)$ in (8.52),

$$z = i\rho = \rho\mathrm{e}^{i\pi/2}, \; \rho = (\upsilon x)^2, \; \bar{z} = \rho\mathrm{e}^{-i\pi/2} = -z, \; \psi(x) = \rho^{1/4\pm\mu}\mathrm{e}^{-z/2}\phi_\pm(z),$$

where μ is given by expression (8.53). Then $\phi_\pm(z)$ satisfy the equations

$$z d_z^2 \phi_\pm(z) + (\beta_\pm - z) d_z \phi_\pm(z) - \alpha_\pm \phi_\pm(z) = 0,$$
$$\alpha_\pm = 1/2 \pm \mu + iw, \ \beta_\pm = 1 \pm 2\mu, \ w = W/4\upsilon^2,$$

which have the confluent hypergeometric functions $\Phi(\alpha_\pm, \beta_\pm; z)$ and $\Psi(\alpha_\pm, \beta_\pm; z)$ as solutions; see [1, 20, 81].

In what follows, we will use the following three solutions of (8.52):

$$u_1(x; W) = \rho^{1/4+\mu} e^{-z/2} \Phi(\alpha, \beta; z), \ \alpha = \alpha_+, \ \beta = \beta_+,$$
$$u_2(x; W) = \rho^{1/4-\mu} e^{-z/2} \Phi(\alpha_-, \beta_-; z),$$
$$V_1(x; W) = \rho^{1/4+\mu} e^{-z/2} \Psi(\alpha, \beta; z) - e^{-i\pi\alpha} \frac{\Gamma(\beta - \alpha)}{\Gamma(\beta)} u_1(x; W)$$
$$= \left[\frac{\Gamma(-2\mu)}{\Gamma(\alpha_-)} - e^{-i\pi\alpha} \frac{\Gamma(\beta - \alpha)}{\Gamma(\beta)} \right] u_1(x; W) + e^{-i\pi\mu} \frac{\Gamma(2\mu)}{\Gamma(\alpha)} u_2(x; W).$$

We note that the functions $u_1(x; W)$ and $V_1(x; W)$ are defined for any values of parameters α and β, whereas $u_2(x; W)$ is defined for $2\mu \neq m \in \mathbb{N}$. All three functions are entire in W. The function $u_1(x; W)$ is real entire in W for $g_1 \geq -1/4$ ($\mu \geq 0$), and $u_2(x; W)$ is real entire in W for $g_1 \geq -1/4$ and $2\mu \neq m \in \mathbb{N}$. If $g_1 < -1/4$ ($\mu = i\varkappa$), then $u_1(x; W)$ and $u_2(x; W)$ are entire in W and $u_2(x; E) = \overline{u_1(x; E)}$.

Below, we list some asymptotics of the introduced functions as $x \to 0$ and $x \to \infty$; see [1, 20, 81].

For $x \to \infty$ ($\rho \to \infty$), we have ($w = a + ib, 0 \leq b < 3/4$)

$$u_1(x; W) = \frac{\Gamma(\beta)}{\Gamma(\beta - \alpha)} e^{i\pi\alpha/2 - i[\rho/2 + a \ln \rho]} (\upsilon x)^{-(1/2 - 2b)}$$
$$+ \frac{\Gamma(\beta)}{\Gamma(\alpha)} e^{i\pi(\alpha - \beta)/2 + i[\rho/2 + a \ln \rho]} (\upsilon x)^{-(1/2 + 2b)} + O\left(x^{-(5/2 - 2b)}\right),$$
$$V_1(x; W) = -\frac{\Gamma(\beta - \alpha)}{\Gamma(\alpha)} e^{-i\pi(\alpha + \beta)/2 + i[\rho/2 + a \ln \rho]} (\upsilon x)^{-(1/2 + 2b)}$$
$$+ O\left(x^{-(5/2 - 2b)}\right).$$

For $x \to 0$ ($\rho \to 0$), we have

$$u_1 = \rho^{1/4+\mu} \tilde{O}(\rho) = (\upsilon x)^{1/2+2\mu} \tilde{O}(x^2) \to 0,$$
$$u_2 = \rho^{1/4-\mu} \tilde{O}(\rho) = (\upsilon x)^{1/2-2\mu} \tilde{O}(x^2), \tag{8.69}$$

and

$$V_1(x;W) = \begin{cases} \mathrm{e}^{-i\pi\mu}\frac{\Gamma(2\mu)}{\Gamma(\alpha)}(\upsilon x)^{1/2-2\mu}\tilde{O}(x^2),\ g_1 > 3/4, \\ -\frac{i}{\Gamma(\alpha)}(\upsilon x)^{-1/2}\tilde{O}(x^2\ln x),\ g_1 = 3/4, \\ \mathrm{e}^{-i\pi\mu}\frac{\Gamma(2\mu)}{\Gamma(\alpha)}(\upsilon x)^{1/2-2\mu} + (\upsilon x)^{1/2+2\mu}\left[\frac{\Gamma(-2\mu)}{\Gamma(\alpha_-)} - \mathrm{e}^{-i\pi\alpha}\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)}\right] \\ +O(x^{5/2-2\mu}),\ g_1 < 3/4,\ g_1 \neq -1/4, \\ -\frac{(\upsilon x)^{1/2}}{\Gamma(\alpha_0)}[c(W) + 2\ln(\upsilon x)] + O(x^{5/2}\ln x),\ g_1 = -1/4, \end{cases} \tag{8.70}$$

where

$$\alpha_0 = 1/2 + iw,\ c(W) = \psi(\alpha_0) - 2\psi(1) + i\pi/2 + \frac{\pi\mathrm{e}^{-i\pi\alpha_0}}{\cos h(\pi w)}. \tag{8.71}$$

Since

$$\mathrm{Wr}\,(u_1, u_2) = -4\mu\upsilon,\ \mathrm{Wr}\,(u_1, V_1) = -2\upsilon\mathrm{e}^{-i\pi\mu}\Gamma(\beta)\Gamma^{-1}(\alpha) = -\omega(W),$$

solutions u_1 and V_1 are linearly independent and form a fundamental set of solutions of (8.52) for $\mathrm{Im}\,W \neq 0$.

We note that for $g_1 \geq 3/4$, the function $V_1\,(x;W)$ is not square-integrable at the origin, whereas for $g_1 < 3/4$ it is (moreover, any solution is square-integrable at the origin). One can see that for $g_1 \geq 3/4$, (8.52) has no square-integrable solutions, and the deficiency indices of the initial symmetric operator $\hat{H}$ are zero, and $\hat{H}_1 = \hat{H}^+$, $D_{H_1} = D^*_{\check{H}}(\mathbb{R}_+)$, is a unique s.a. extension of $\hat{H}$. For $g_1 < 3/4$ there is one square-integrable solution, $V_1\,(x;W)$, and the deficiency indices of $\hat{H}$ are $m_\pm = 1$. Moreover, one can easily see that the discrete spectrum is absent.

The majority of results obtained in range A, such as a description of the natural domain, can be used without any modification in the present range B. We shall use these results below.

8.4.2.1 Subrange $g_1 \geq 3/4$

For such g_1, the unique s.a. extension of $\hat{H}$ is $\hat{H}_1 = \hat{H}^+$. The Green's function and the derivative of the spectral function have the forms (8.60) and (8.61) respectively. The same guiding functional as in the range A allows one to conclude that the spectrum of $\hat{H}_1$ is simple.

In the range $m - 1 < 2\mu < m + 1$, $m \in \mathbb{N}$, the function $V_1(x;W)$ can be represented as

$$V_1(x;W) = A_m(W)u_1(x;W) + \frac{\omega(W)}{4\mu\upsilon}V_{(m)}(x;W),$$

$$A_m(W) = \frac{\Gamma(-2\mu)}{\Gamma(\alpha_-)} + \frac{\mathrm{e}^{i(\pi/2)(m-2\mu)}\Gamma(2\mu)\Gamma(\beta_-)\Gamma(\alpha_m)}{m!\Gamma(\alpha)\Gamma(\alpha_{-m})}$$
$$-\mathrm{e}^{-i\pi\alpha}\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)},\ V_{(m)}(x;W) = u_2\,(x;W)$$
$$-\frac{\mathrm{e}^{i\pi m/2}\Gamma(\alpha_m)\Gamma(\beta_-)}{m!\Gamma(\alpha_{-m})}u_1\,(x;W)\,,\ \alpha_{\pm m} = 1/2 \pm m/2 + iw.$$

One can see that the function $A_m(W)$ is well defined for any W and for $m - 1 < 2\mu < m + 1$, and is analytic in a neighborhood of the real axis (at least for $|b| < 1/2$), and the function $V_{(m)}(x;W)$ is real entire in W. As a result, we obtain

$$\sigma'(E) = \frac{\mathrm{e}^{\pi E/4\upsilon^2}|\Gamma(1/2+\mu+iE/4\upsilon^2)|^2}{4\pi\upsilon\Gamma^2(\beta)} > 0.$$

Thus, the simple spectrum of $\hat{H}_1$ has the form spec $\hat{H}_1 = \mathbb{R}$, and the generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_1(x;E)$ of $\hat{H}_1$ form a complete orthonormalized system in $L^2\,(\mathbb{R}_+)$.

8.4.2.2 Subrange $3/4 > g_1 > -1/4$ $(1/2 > \mu > 0)$

Using the asymptotics (8.57), we obtain $\Delta_{H^+}(\psi_*) = -4\mu\upsilon(\overline{c_1}c_2 - \overline{c_2}c_1)$, which means that deficiency indices of $\check{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $c_1\cos\nu = c_2\sin\nu$, $\nu \in \mathbb{S}(-\pi/2,\pi/2)$. Thus, in the subrange under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{2,\nu}$ parameterized by ν with domains $D_{H_{2\nu}}$,

$$D_{H_{2\nu}} = \{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ obey } (8.62)\}.$$

Imposing the boundary conditions (8.62) on the functions (8.59), using the asymptotics (8.69), (8.70), and representing the function $V_1(x;W)$ in the form

$$V_1(x;W) = \frac{1}{2\mu}\left[A(W)u_{2,\nu}(x;W) - B(W)\tilde{u}_{2,\nu}(x;W)\right],$$
$$u_{2,\nu}(x;W) = u_1(x;W)\sin\nu + u_2(x;W)\cos\nu,$$
$$\tilde{u}_{2,\nu}(x;W) = u_1(x;W)\cos\nu - u_2(x;W)\sin\nu,$$

where

$$A(W) = -a(W)\sin\nu + b(W)\cos\nu,\ B(W) = a(W)\cos\nu + b(W)\sin\nu,$$
$$a(W) = \frac{\Gamma(\beta_-)}{\Gamma(\alpha_-)} + \mathrm{e}^{-i\pi\alpha}\frac{\Gamma(\beta-\alpha)}{\Gamma(2\mu)},\ \ b(W) = \mathrm{e}^{-i\pi\mu}\frac{\Gamma(\beta)}{\Gamma(\alpha)},$$

we obtain the Green's function of the Hamiltonian $\hat{H}_{2\nu}$,

$$G(x, y; W) = \frac{1}{4\mu\upsilon}\left[\frac{A(W)}{B(W)}u_{2,\nu}(x; W)u_{2,\nu}(y; W) - \left\{\begin{array}{l}\tilde{u}_{2,\nu}(x; W)u_{2,\nu}(y; W),\ x > y,\\ u_{2,\nu}(x; W)\tilde{u}_{2,\nu}(y; W),\ x < y\end{array}\right.\right], \tag{8.72}$$

where the second term on the right-hand side of (8.72) is real for real $W = E$.

We note that the functions $u_{2,\nu}(x; W)$ and $\tilde{u}_{2,\nu}(x; W)$ are solutions of (8.52) real entire in W and $u_{2,\nu}(x; W)$ satisfies the boundary condition (8.62).

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_{2,\nu}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{2\nu}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{2,\nu}$ ($\tilde{U} = \tilde{u}_{2,\nu}$), and therefore the spectra of $\hat{H}_{2\nu}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function,

$$\sigma'(E) = \frac{(4\pi\mu\upsilon)^{-1}\left|\Gamma(\alpha)\right|^{-2}2\Gamma(2\mu)\Gamma(\beta)\sin^2(2\pi\mu)\mathrm{e}^{\pi E/4\upsilon^2}}{\left\{[\mathrm{e}^{\pi E/4\upsilon^2}\cos(2\pi\mu) + \mathrm{e}^{-\pi E/4\upsilon^2}]\cos\nu + \tilde{\nu}\right\}^2 + \mathrm{e}^{2\pi E/4\upsilon^2}\sin^2(2\pi\mu)\cos^2\nu},$$

$$\tilde{\nu} = |\Gamma(\alpha)|^{-2}\Gamma(2\mu)\Gamma(\beta)\sin(2\pi\mu)\sin\nu.$$

Because $\sigma'(E) > 0$, the simple spectrum of $\hat{H}_{2\nu}$ has the form $\operatorname{spec}\hat{H}_{2\nu} = \mathbb{R}$. The generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_{2,\nu}(x; E)$ of $\hat{H}_{2\nu}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

One can see that for $\nu = \pm\pi/2$, all the results coincide with those of the previous subrange for g_1.

8.4.2.3 Subrange $g_1 = -1/4$ ($\mu = 0$)

Using the asymptotics (8.57), we obtain $\Delta_{H^+}(\psi_*) = 2\upsilon(\overline{c_1}c_2 - \overline{c_2}c_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $c_1\cos\vartheta = c_2\sin\vartheta$, $\vartheta \in \mathbb{S}(-\pi/2, \pi/2)$. Thus, in the subrange under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{3\vartheta}$ parameterized by ϑ with domains $D_{H_{3\vartheta}}$,

$$D_{H_{3\vartheta}} = \left\{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy } (8.64)\right\}.$$

Imposing the boundary conditions (8.64) on the functions (8.59), using the asymptotics (8.69), (8.70), and representing the function $-\Gamma(\alpha_0)V_1(x;W)$ as

$$
\begin{aligned}
-\Gamma(\alpha)V_1(x;W) &= A(W)u_{3,\vartheta}(x;W) + B(W)\tilde{u}_{3,\vartheta}(x;W),\\
u_{3,\vartheta}(x;W) &= u_1(x;W)\sin\vartheta + u_3(x;W)\cos\vartheta,\\
\tilde{u}_{3,\vartheta}(x;W) &= u_1(x;W)\cos\vartheta - u_3(x;W)\sin\vartheta,\\
u_3(x;W) &= -c(W)u_1(x;W) - \Gamma(\alpha_0)V_1(x;W)\\
&= \partial_\mu\left[\rho^{1/4+\mu}\mathrm{e}^{-z/2}\Phi(1/2+\mu+iw, \beta_\pm = 1+2\mu; z)\right]\Big|_{\mu=0},\\
A(W) &= c(W)\sin\vartheta + \cos\vartheta,\ B(W) = c(W)\cos\vartheta - \sin\vartheta,
\end{aligned}
$$

where $c(W)$ is given in (8.71), we obtain the Green's function of the Hamiltonian $\hat{H}_{3\vartheta}$,

$$
\begin{aligned}
G(x,y;W) = \frac{1}{2\upsilon}\Bigg[&\frac{A(W)}{B(W)}u_{3,\vartheta}(x;W)u_{3,\vartheta}(y;W)\\
&+\begin{cases}\tilde{u}_{3,\vartheta}(x;W)u_{3,\vartheta}(y;W), & x>y,\\ u_{3,\vartheta}(x;W)\tilde{u}_{3,\vartheta}(y;W), & x<y\end{cases}\Bigg],
\end{aligned}
\tag{8.73}
$$

where the second term on the right-hand side of (8.73) is real for real $W = E$.

We note that the functions $u_{3,\vartheta}(x;W)$ and $\tilde{u}_{3,\vartheta}(x;W)$ are solutions of (8.52) real entire in W, and $u_{3,\vartheta}(x;W)$ satisfies the boundary condition (8.64).

Consider the guiding functional

$$
\Phi(\xi;W) = \int_0^\infty \mathrm{d}x u_{3,\vartheta}(x;W)\xi(x),\ \xi\in\mathcal{D}_r(\mathbb{R}_+)\cap D_{H_{3\vartheta}}.
$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{3,\vartheta}$ ($\tilde{U} = \tilde{u}_{3,\vartheta}$), and therefore the spectra of $\hat{H}_{3\vartheta}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function,

$$
\begin{aligned}
&\sigma'(E)\\
&= \frac{(4\upsilon)^{-1}\left[1+\tan h(\pi E/4\upsilon^2)\right]}{\left\{\left[\operatorname{Re}\psi(\alpha_0) - 2\psi(1)\right]\cos\vartheta - \sin\vartheta\right\}^2 + (\pi^2/4)\left[1+\tan h\left(\pi E/4\upsilon^2\right)\right]^2\cos^2\vartheta}.
\end{aligned}
$$

Because $\sigma'(E) > 0$, the simple spectrum of $\hat{H}_{3\vartheta}$ has the form spec $\hat{H}_{3\vartheta} = \mathbb{R}$. The generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_{3,\vartheta}(x;E)$ of $\hat{H}_{3\vartheta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. Note that for $\vartheta = \pm\pi/2$, all the results coincide with those of the range $g_1 \geq 3/4$ in the limit $\mu = 0$, i.e., in the limit $g_1 \to -1/4$.

8.4.2.4 Subrange $g_1 < -1/4$ ($\mu = i\varkappa$, $\varkappa > 0$)

Using the asymptotics (8.57), we obtain $\Delta_{H+}(\psi_*) = -4i\varkappa\upsilon(\overline{c_1}c_2 - \overline{c_2}c_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H+}(\psi_*) = 0$ implies $c_1 = \mathrm{e}^{2i\theta}c_2$, $\theta \in \mathbb{S}(0,\pi)$. Thus, in the subrange under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{4\theta}$ parameterized by θ with domains

$$D_{H_{4\theta}} = \{\psi : \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy (8.67)}\}.$$

Imposing the boundary conditions (8.67) on the functions (8.59), using the asymptotics (8.69), (8.70), and representing the function $V_1(x;W)$ in the form

$$\begin{aligned}
V_1(x;W) &= -\frac{1}{4\varkappa}\left[A(W)u_{4,\theta}(x;W) + B(W)\tilde{u}_{4,\theta}(x;W)\right],\\
u_{4,\theta}(x;W) &= \mathrm{e}^{i\theta}u_1(x;W) + \mathrm{e}^{-i\theta}u_2(x;W),\\
\tilde{u}_{4,\theta}(x;W) &= i\,[\mathrm{e}^{-i\theta}u_2(x;W) - \mathrm{e}^{i\theta}u_1(x;W)],\\
A(W) &= i\left[\mathrm{e}^{i\theta}b(W) - \mathrm{e}^{-i\theta}a(W)\right],\ B(W) = \mathrm{e}^{i\theta}b(W) + \mathrm{e}^{-i\theta}a(W),
\end{aligned}$$

where $u_{4,\theta}(x;W)$ and $\tilde{u}_{4,\theta}(x;W)$ are real entire solutions of (8.52) and $u_{4,\theta}(x;W)$ satisfies the boundary conditions (8.67), we obtain the Green's function of the Hamiltonian $\hat{H}_{4\theta}$,

$$\begin{aligned}
G(x,y;W) = -\frac{1}{8\varkappa\upsilon}\Bigg[&\frac{A(W)}{B(W)}u_{4,\theta}(x;W)u_{4,\theta}(y;W)\\
&+\begin{cases}\tilde{u}_{4,\theta}(x;W)u_{4,\theta}(y;W),\ x > y,\\ u_{4,\theta}(x;W)\tilde{u}_{4,\theta}(y;W),\ x < y\end{cases}\Bigg],
\end{aligned} \tag{8.74}$$

where the second term on the right-hand side of (8.74) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x\, u_{4,\theta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{4\theta}}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = u_{4,\theta}$ ($\tilde{U} = \tilde{u}_{4,\theta}$), and therefore the spectra of $\hat{H}_{4\theta}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function,

$$\begin{aligned}
\sigma'(E) &= \frac{1}{8\pi\varkappa\upsilon}\frac{D(E)\bar{D}(E) - 1}{|D(E)+1|^2} > 0,\ D(E)\bar{D}(E) = |D(E)|^2,\\
D(E) &= \mathrm{e}^{-2i\theta}\frac{a(E)}{b(E)},\ |D(E)| = \mathrm{e}^{\pi\varkappa}\left(\frac{\cos h[\pi(\varkappa + E/4\upsilon^2)]}{\cos h[\pi(\varkappa - E/4\upsilon^2)]}\right)^{1/2} > 1.
\end{aligned}$$

Thus, the simple spectra of $\hat{H}_{4\theta}$ have the form spec $\hat{H}_{4\theta} = \mathbb{R}$ and the generalized eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}u_{4,\theta}(x; E)$ of $\hat{H}_{4\theta}$ form a complete orthonormalized systems in $L^2(\mathbb{R}_+)$.

The main conclusion is that for the ESP IV under consideration, with $g_2 < 0$, the spectrum of any s.a. Schrödinger operator is simple, continuous, unbounded from below, and all the points of the real axis $\mathbb{R}$ belong to the spectrum.

8.5 ESP V

In this case,

$$V(x) = g_1 \mathrm{e}^{-2cx} + g_2 \mathrm{e}^{-cx}, \quad x \in \mathbb{R}, \tag{8.75}$$

and the corresponding Schrödinger equation is

$$\psi'' - \left(g_1 \mathrm{e}^{-2cx} + g_2 \mathrm{e}^{-cx}\right)\psi + W\psi = 0. \tag{8.76}$$

It is sufficient to consider only the case $c > 0$, because the case with $c < 0$ is reduced to the former one by the transformation $x \to -x$.

The potential (8.75) is known as the *Morse potential*; see [113]. Such a potential was suggested to explain the observed vibrational energy levels and dissociation energies of diatomic molecules. It has been also applied to the deuteron problem [114].

Below, we consider separately three ranges: $g_1 = \upsilon^2 > 0$, $\upsilon > 0$; $g_1 = -\upsilon^2 < 0$, $\upsilon > 0$; and $g_1 = 0$.

8.5.1 Range 1

In this range, we have

$$g_1 = \upsilon^2 > 0, \ \upsilon > 0.$$

Here, we introduce a new variable $z \in \mathbb{R}_+$ and a new function ϕ, instead of x and $\psi(x)$ in (8.76),

$$\begin{aligned}
&z = 2\upsilon c^{-1}\mathrm{e}^{-cx}, \ x = -c^{-1}\ln\left(\frac{cz}{2\upsilon}\right), \ \psi(x) = z^{\mu}\mathrm{e}^{-z/2}\phi(z), \\
&\mu = c^{-1}(-W)^{1/2} = c^{-1}|W|^{1/2}(\sin\varphi/2 - i\cos\varphi/2), \\
&\operatorname{Re}\mu \geq 0; \ \operatorname{Re}\mu > 0 \text{ for } \operatorname{Im}W > 0,
\end{aligned} \tag{8.77}$$

where $W = |W|\mathrm{e}^{i\varphi}$, $0 \leq \varphi \leq \pi$. Then $\phi(z)$ obeys the equation

$$z d_z^2\phi(z) + (1 + 2\mu - z)d_z\phi(z) - (1/2 + \mu + q)\phi(z) = 0,$$

where $q = g_2/2c\upsilon$. This equation has the confluent hypergeometric functions $\Phi(\alpha, \beta; z)$ and $\Psi(\alpha, \beta; z)$ (with $\alpha = 1/2 + \mu + q$, $\beta = 1 + 2\mu$) as solutions; see [1, 20, 81].

In what follows, we use the following two solutions of (8.76):

$$\begin{aligned}
u_1(x; W) &= z^\mu e^{-z/2}\Psi(\alpha, \beta; z) \\
&\qquad = \frac{\pi e^{-z/2}}{\sin(2\pi\mu)}\left(\frac{z^{-\mu}\Phi(\alpha_-, \beta_-; z)}{\Gamma(\alpha)\Gamma(\beta_-)} - \frac{z^\mu \Phi(\alpha, \beta; z)}{\Gamma(\alpha_-)\Gamma(\beta)}\right), \\
u_2(x; W) &= \frac{z^\mu e^{-z/2}}{\Gamma(\beta)}\Phi(\alpha, \beta; z), \\
\alpha_- &= \alpha - \beta + 1 = 1/2 - \mu + q,\ \beta_- = 2 - \beta = 1 - 2\mu,\ \mathrm{Re}\,\beta \geq 1.
\end{aligned}$$

We note that $u_1(x; W)$ and $u_2(x; W)$ are defined for any α and β, $u_1(x; W)$ is real entire in W, and $u_2(x; E + i0)$ is real for $E \leq 0$.

Below, we list some asymptotics as $|x| \to \infty$ of the introduced functions; see [1, 20, 81].

For $x \to \infty$ $(z \to 0)$, $\mathrm{Im}\, W > 0$, we have

$$\begin{aligned}
u_1 &= \frac{\Gamma(\beta)(2\upsilon/c)^{-\mu}}{2\mu\Gamma(\alpha)} e^{|W|^{1/2}[-ix\cos(\varphi/2) + x\sin(\varphi/2)]}\tilde{O}\left(e^{-cx}\right) \\
&= O\left(e^{x|W|^{1/2}\sin(\varphi/2)}\right) \to \infty, \\
u_2 &= \frac{(2\upsilon/c)^\mu}{\Gamma(\beta)} e^{|W|^{1/2}[ix\cos(\varphi/2) - x\sin(\varphi/2)]}\tilde{O}\left(e^{-cx}\right) \\
&= O\left(e^{-x|W|^{1/2}\sin(\varphi/2)}\right) \to 0.
\end{aligned}$$

For $x \to -\infty$ $(z \to \infty)$, we have

$$\begin{aligned}
u_1 &= e^{-z/2} z^{-1/2 - g_2/(2c\upsilon)}\tilde{O}(z^{-1}) \\
&= O\left[e^{-(\upsilon/c)e^{c|x|}} e^{-(g_2/(c\upsilon) + c)|x|/2}\right] \to 0, \\
u_2 &= \Gamma^{-1}(\alpha) e^{z/2} z^{-1/2 + g_2/(2c\upsilon)}\tilde{O}(z^{-1}) \\
&= O\left[e^{(\upsilon/c)e^{c|x|}} e^{(g_2/(c\upsilon) - c)|x|/2}\right] \to \infty.
\end{aligned}$$

Since $\mathrm{Wr}(u_1, u_2) = -c/\Gamma(\alpha)$, the solutions u_1 and u_2 are linearly independent and form a fundamental set of solutions of (8.76) for $\mathrm{Im}\, W \neq 0$.

One can see that for $\mathrm{Im}\, W \neq 0$, any linear combination of the fundamental set is not square-integrable. The latter means that the deficient subspaces are empty and both deficiency indices are zero.

We note that $u_1 \in L^2(-\infty, x_0)$ and $u_2 \in L^2(x_0, \infty)$ for any finite x_0 and $\operatorname{Im} W > 0$. This fact will be used in constructing Green's functions.

As usual, starting with the s.a. differential operation $\check{H}$ with the potential (8.76), we construct the initial symmetric operator $\hat{H}$ defined on the domain $\mathcal{D}(\mathbb{R})$. Its adjoint $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R})$. Taking into account that in the case under consideration $[\psi_*, \psi_*](x) \overset{|x|\to\infty}{\longrightarrow} 0$, $\forall \psi_* \in D^*_{\check{H}}(\mathbb{R})$, see Sect. 7.1, we calculate the asymmetry form $\Delta_{H^+}(\psi_*)$ to obtain

$$\Delta_{H^+}(\psi_*) = [\psi_*, \psi_*]|_{-\infty}^{\infty} = 0, \quad \forall \psi_* \in D^*_{\check{H}}(\mathbb{R}).$$

This result implies that the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

To construct the Green's function of the operator $\hat{H}_1$, we consider, following Sect. 5.3.2, the general solution of the inhomogeneous equation

$$\left(\check{H} - W\right)\psi = \eta \in L^2(\mathbb{R}), \ \operatorname{Im} W > 0.$$

Such a solution has the form

$$\psi(x) = c_1 u_1(x; W) + c_2 u_2(x; W) + \frac{\Gamma(\alpha)}{c}\Big[u_2(x; W) \times \int_{-\infty}^{x} u_1(y; W)\eta(y)\mathrm{d}y + u_1(x; W)\int_{x}^{\infty} u_2(y; W)\eta(y)\mathrm{d}y\Big],$$

where $c_{1,2}$ are arbitrary constants. By the help of the Cauchy–Schwarz inequality, we can see that both terms in square brackets are bounded as $|x| \to \infty$, which implies $c_1 = c_2 = 0$ for functions ψ to be square-integrable. Then the Green's function of the operator $\hat{H}_1$ has the form

$$\begin{aligned} G(x, y; W) &= \frac{\Gamma(\alpha)}{c}\begin{cases} u_2(x; W)u_1(y; W), & x > y \\ u_1(x; W)u_2(y; W), & x < y \end{cases} \\ &= \frac{\lambda(W)}{c}\Bigg[-\frac{\Gamma(\alpha)\sin(2\pi\mu)}{\pi}u_1(x; W)u_1(x; W) \\ &\quad + \begin{cases} u_3(x; W)u_1(y; W), & x > y, \\ u_1(x; W)u_3(y; W), & x < y \end{cases}\Bigg], \end{aligned}$$

where

$$\lambda(W) = \frac{\Gamma(\alpha)\Gamma(\alpha_-)}{\Gamma(\alpha) + \Gamma(\alpha_-)},$$

$$u_3 = \mathrm{e}^{-z/2}\left[\frac{z^{\mu}}{\Gamma(\beta)}\Phi(\alpha, \beta; z) + \frac{z^{-\mu}}{\Gamma(\beta_-)}\Phi(\alpha_-, \beta_-; z)\right].$$

We note that $u_3(x; W)$ is a solution of (8.76) real entire in W.

Consider a guiding functional

$$\Phi\left(\xi;W\right)=\int_{\mathbb{R}}\mathrm{d}x\,u_1\left(x;W\right)\xi\left(x\right),\ \xi\in\mathbb{D}=D_r\left(\mathbb{R}\right)\cap D^*_{\check{H}}\left(\mathbb{R}\right). \tag{8.78}$$

The space $\mathbb{D}$ is dense in $L^2(\mathbb{R})$ owing to $\mathcal{D}(\mathbb{R})\subset\mathbb{D}$. Properties (i) and (iii) of Sect. 5.3.3 are obviously fulfilled, and we have only to check Property (ii).

Let there exist $\xi_0(x)\in\mathbb{D}$ and $E_0\in\mathbb{R}$ such that

$$\Phi\left(\xi_0;E_0\right)=\int_{-\infty}^{b}\mathrm{d}x\,u_1\left(x;E_0\right)\xi_0\left(x\right)=0,\ \mathrm{supp}\xi_0\in(-\infty,b].$$

Let us consider a solution

$$\psi(x)=u\left(x;E_0\right)\int_{-\infty}^{x}u_1\left(y;E_0\right)\xi_0\left(y\right)\mathrm{d}y+u_1\left(x;E_0\right)\int_{x}^{\infty}u\left(y;E_0\right)\xi_0\left(y\right)\mathrm{d}y$$

of the equation $(\check{H}-E_0)\psi=\xi_0$, where $u;(x;W)$ is an arbitrary solution of (8.76) satisfying the condition $\mathrm{Wr}(u,u_1)=1$. Using the Cauchy–Schwarz inequality, we can prove[2] that

$$\psi(x)=O(z^{-3/2})=O(\mathrm{e}^{-3c|x|/2}),\ x\to-\infty,$$

so that $\psi,\check{H}\psi=\xi_0+E_0\psi\in L^2(\mathbb{R})$. Thus, $\psi\in\mathbb{D}$, and therefore $\Phi\left(\xi;W\right)$ is a simple guiding functional, so that the spectrum of $\hat{H}_1$ is simple.

With the help of (5.22), we obtain

$$\begin{aligned}&\pi c u_1\left(x_0;E\right)\sigma'\left(E\right)=\mathrm{Im}[\Gamma(\alpha)u_2\left(x_0;W\right)]_{W=E+i0}=-\pi^{-1}u_1\left(x_0;E\right)\\&\times\mathrm{Im}[\Gamma(\alpha)\sin(2\pi\mu)\lambda(W)]_{W=E+i0}+u_3\left(x_0;E\right)\mathrm{Im}\,\lambda(E+i0).\end{aligned} \tag{8.79}$$

1. Consider the case $1/2+q\notin\mathbb{Z}_-$.

   (a) Let $E=c^2p^2\geq 0$ and

   $$\mu=-ip,\ p\geq 0,\ \alpha=1/2+q-ip,\ \alpha_-=1/2+q+ip,\ \beta=1-2ip.$$

   Then $\Gamma(\alpha_-)=\overline{\Gamma(\alpha)}$, $\Gamma(\alpha)\neq\infty$. If $\mathrm{Re}\,\Gamma(\alpha)\neq 0$, then $\lambda(E\geq 0)$ is finite and real, so that it follows from the second line in (8.79) that

   $$\sigma'\left(E\right)=\frac{\sin h(2\pi p)\lambda(E)}{\pi^2 c}\mathrm{Re}\,\Gamma(\alpha)=\frac{\sin h(2\pi p)}{2\pi^2 c}|\Gamma(\alpha)|^2.$$

---

[2] For estimating integrals, it is convenient to pass from integration over x to integration over z.

If $\operatorname{Re}\Gamma(\alpha) = 0$, then

$$u_1(x_0; E) = 2\pi\,[\sin h(2\pi p)\operatorname{Im}\Gamma(\alpha)]^{-1}\operatorname{Re}u_2(x_0; E),$$

and it follows from the first line in (8.80) that

$$\sigma'(E) = \frac{\sin h(2\pi p)\,[\operatorname{Im}\Gamma(\alpha)]^2}{2\pi^2 c\operatorname{Re}u_2(x_0; E)}\operatorname{Im}[iu_2(x_0; E)] = \frac{\sin h(2\pi p)}{2\pi^2 c}|\Gamma(\alpha)|^2.$$

Finally, we obtain that

$$\sigma'(E) = \frac{\sin h(2\pi p)}{2\pi^2 c}|\Gamma(\alpha)|^2 > 0,\ E \geq 0,$$

which means that spec $\hat{H}_1 = \mathbb{R}_+$.

(b) Let $E = -c^2\tau^2 < 0$. Then

$$\mu = \tau > 0,\ \alpha = 1/2 + q + \tau,\ \beta = 1 + 2\tau.$$

Here, we find from the first line in (8.79) that

$$\sigma'(E) = \frac{u_2(x_0; E)}{\pi c u_1(x_0; E)}\operatorname{Im}\Gamma(\alpha)_{W=E+i0},$$

where we recall that $u_1(x_0; E)$ and $u_2(x_0; E)$ are real. Because $\Gamma(\alpha)|_{W=E}$ is real if $\Gamma(\alpha)|_{W=E}$ is finite, it follows that $\operatorname{Im}\Gamma(\alpha)$ and $\sigma'(E)$ differ from zero only at the points E_n for which $|\Gamma(\alpha)| = \infty$. At these points, $\alpha = \alpha_n = 1/2 + q + \tau_n = -n$, $n \in \mathbb{Z}_+$, so that

$$E_n = -c^2(1/2 + n + q)^2,\ n \in \mathbb{Z}_+.$$

If $g_2 < -c\upsilon$, and there exists a natural number $n_{\max} \in \mathbb{Z}_+$ such that

$$c\upsilon(1 + 2n_{\max}) < |g_2| < c\upsilon(3 + 2n_{\max}),$$

then there exist $n_{\max} + 1$ discrete levels

$$E_n = -c^2(|q| - n - 1/2)^2,\ \ n = 0, 1, \ldots, n_{\max}.$$

For $\alpha = \alpha_n = -n$, we have

$$u_2(x_0; E_n) = (-1)^n\Gamma^{-1}(2|q| - n)u_1(x_0; E_n).$$

Using relations

$$\alpha|_{W=E+i\varepsilon} = -n - \frac{\tilde{\Delta}}{2c\sqrt{|E_n|}} + O(\tilde{\Delta}^2),\ \tilde{\Delta} = E - E_n + i\varepsilon,$$

$$\operatorname{Im}\Gamma(\alpha) = (-1)^n\frac{2\pi c\sqrt{|E_n|}}{n!}\delta(E - E_n),$$

for E in a neighborhood of E_n, see Lemma 5.17, we obtain

$$\sigma'(E) = \sum_{n=0}^{n_{\max}} Q_n^2 \delta(E - E_n),\ Q_n = \sqrt{\frac{2\sqrt{|E_n|}}{n!\Gamma(2|q| - n)}}.$$

2. Consider the case $1/2 + q = -l$, $l \in \mathbb{Z}_+$, i.e., $g_2 = -c\upsilon(1 + 2l)$.

(a) Let $E \neq 0$. Then all the above considerations and conclusions hold, and in particular, there exist l discrete energy levels $E_n \neq 0$, $n = 0, 1, \ldots, l - 1$.

(b) Suppose E is situated in a neighborhood of $E = 0$. Here $\mu \sim 0$, and

$$\Gamma(\alpha) = \frac{(-1)^l}{\mu l!},\ u_2(x; 0) = \mathrm{e}^{-z/2}\Phi(-l, 1; z),\ u_1(x; 0) = (-1)^l l! u_2(x; 0),$$

so that

$$\sigma'(E) = \left[\pi(l!)^2\right]^{-1} \mathrm{Im}[-(E + i0)]^{-1/2} = \begin{cases} \left[\pi(l!)^2\sqrt{E}\right]^{-1},\ E > 0, \\ 0,\ E < 0, \end{cases}$$

$$\sigma(E) = \begin{cases} 2\sqrt{E}\left[\pi(l!)^2\right]^{-1},\ E \geq 0, \\ 0,\ E < 0. \end{cases}$$

Because $\sigma(E)$ has a square-root singularity at $E = 0$, there is no discrete level at this point. This conclusion can be justified by a direct solution of (8.76) with $W = 0$. Its unique solution square-integrable on $-\infty$ is

$$\psi(x) = C\mathrm{e}^{-z/2}\Psi(\alpha, 1; z),\ \alpha = 1/2 + q.$$

As $x \to \infty$, we obtain

$$\psi(x) \to \begin{cases} \Gamma^{-1}(\alpha)cx,\ \alpha \notin \mathbb{Z}_-, \\ (-1)^n n!,\ \alpha = -n,\ n \in \mathbb{Z}_+. \end{cases}$$

This means that there exists no square-integrable solution of (8.76) with zero energy.

Finally, we obtain for the simple spectrum of $\hat{H}_1$,

$$\operatorname{spec} \hat{H}_1 = \begin{cases} \mathbb{R}_+,\ g_2 \geq -c\upsilon, \\ \mathbb{R}_+ \cup \{E_n\},\ n = 0, 1, \ldots, n_{\max},\ n_{\max} \in \mathbb{Z}_+, \\ -c\upsilon(1 + 2k) > g_2 \geq -c\upsilon(3 + 2k). \end{cases}$$

The (generalized) eigenfunction $U_E(x) = \sqrt{\sigma'(E)} u_1(x; E)$, $E \geq 0$, and $U_n(x) = Q_n u_1(x; E_n)$ of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R})$.

We note that $U_n(x)$ are really eigenfunctions of $\hat{H}_1$. Indeed, for $\alpha = -n$, $n \in \mathbb{Z}_+$, we have

$$U_n\,(x) = -\frac{\pi \mathrm{e}^{-z/2} z^{\tau_n} \Phi(-n,\beta;z)}{\sin(2\pi\tau_n)\Gamma(\alpha_-)\Gamma(\beta)}$$

and $\Phi(-n,\beta;z)$ is a polynomial, so that $U_n\,(x) \in L^2(\mathbb{R})$.

8.5.2 Range 2

In this range, we have

$$g_1 = -\upsilon^2 < 0,\ \upsilon > 0.$$

Here, we introduce new variables z_ξ and new functions $\phi_{\pm,\xi}$, instead of x and $\psi\,(x)$ in (8.76),

$$z_\xi = i\xi\rho = \mathrm{e}^{i\xi\pi/2}\rho,\ \rho = 2\upsilon c^{-1}\mathrm{e}^{-cx},\ \rho \in \mathbb{R}_+,\ \xi = \pm 1,$$
$$\psi = \mathrm{e}^{-z_\xi/2} z_\xi^{\pm\mu} \phi_{\pm,\xi}\left(z_\xi\right),$$

where μ is defined in (8.77). Then $\phi_\xi\left(z_\xi\right)$ satisfy the equation

$$z_\xi d_{z_\xi}^2 \phi_{\pm,\xi}\left(z_\xi\right) + (1 \pm 2\mu - z_\xi) d_{z_\xi} \phi_{\pm,\xi}\left(z_\xi\right) - (1/2 \pm \mu - i\xi q)\, \phi_{\pm,\xi}\left(z_\xi\right) = 0,$$

which has the confluent hypergeometric functions Φ and Ψ as solutions; see [1, 20, 81].

In our considerations, we will use different sets of solutions of (8.76). The first of them is

$$P(x;W) = \Gamma^{-1}(\beta)\mathrm{e}^{-z/2} z^\mu \Phi(\alpha,\beta;z),$$
$$P_-(x;W) = \Gamma^{-1}(\beta_-)\mathrm{e}^{-z/2} z^{-\mu} \Phi(\alpha_-,\beta_-;z) = \left. P(x;W)\right|_{\mu\to-\mu},$$
$$\alpha = \alpha_{+|+},\ \alpha_- = \alpha_{-|+},\ \beta = \beta_+,\ \alpha_{\pm|\xi}{=}1/2 \pm \mu - i\xi q,\ \beta_\pm{=}1 \pm 2\mu,\ z{=}z_+.$$

The second set reads

$$u_1\,(x;W) = \mathrm{e}^{-z/2} z^\mu \Psi(\alpha,\beta;z) = \frac{\pi}{\sin(2\pi\mu)}\left(\frac{P_-(x;W)}{\Gamma(\alpha)} - \frac{P(x;W)}{\Gamma(\alpha_-)}\right),$$
$$u_2\,(x;W) = \mathrm{e}^{-z_-/2} z_-^\mu \Psi(\alpha_{+|-},\beta;z_-)$$
$$= \frac{\pi}{\sin(2\pi\mu)}\left(\frac{\mathrm{e}^{i\pi\mu} P_-(x;W)}{\Gamma(\alpha_{+|-})} - \frac{\mathrm{e}^{-i\pi\mu} P(x;W)}{\Gamma(\alpha_{-|-})}\right).$$

And the third set has the form

$$U_\theta(x;W) = e^{i\theta}u_1(x;W) + e^{-i\theta}u_2(x;W), \tag{8.80}$$
$$\tilde{U}_\theta(x;W) = i\left[e^{-i\theta}u_2(x;W) - e^{i\theta}u_1(x;W)\right].$$

There exist relations between functions from different sets:

$$P(x;W) = \frac{i e^{\pi q}e^{i\pi\mu}}{\Gamma(\alpha_{+|-})}u_1(x;W) - \frac{i e^{\pi q}}{\Gamma(\alpha)}u_2(x;W)$$
$$= \frac{i e^{\pi q}}{2}b_\theta(\mu)U_\theta(x;W) - \frac{e^{\pi q}}{2}a_\theta(\mu)\tilde{U}_\theta(x;W),$$
$$b_\theta(\mu) = \frac{e^{-i\theta+i\pi\mu}}{\Gamma(\alpha_{+|-})} - \frac{e^{i\theta}}{\Gamma(\alpha)},\ a_\theta(\mu) = \frac{e^{-i\theta+i\pi\mu}}{\Gamma(\alpha_{+|-})} + \frac{e^{i\theta}}{\Gamma(\alpha)}. \tag{8.81}$$

We note that solutions P, P_-, u_1, and u_2 are defined for any $\alpha_{\pm|\xi}$ and β; $u_{1,2}(x;W)$ are even entire functions of μ and therefore are entire in W;

$$\overline{u_1(x;W)} = u_2\left(x;\overline{W}\right),\ \overline{u_1(x;E)} = u_2(x;E);$$

$P(x;W)$ and $P_-(x;W)$ are analytic functions in $\mathbb{C}_\pm$ with respect to W; the functions $U_\theta(x;W)$ and $\tilde{U}_\theta(x;W)$ are real entire in W.

Below, we list some asymptotics of the introduced functions as $|x| \to \infty$; see [1, 20, 81].

For $x \to -\infty$ ($\rho \to \infty$), we have

$$u_1(x;W) = u_{as}(x) + O\left(e^{-3|x|/2}\right),\ u_2(x;W) = \overline{u_{as}(x)} + O\left(e^{-3|x|/2}\right),$$
$$P(x;W) = i\left[\frac{e^{i\pi\mu+\pi q}}{\Gamma(\alpha_{+|-})}u_{as}(x) - \frac{e^{\pi q}}{\Gamma(\alpha)}\overline{u_{as}(x)}\right] + O\left(e^{-3|x|/2}\right),\ \forall W,$$

where $u_{as}(x) = \tilde{u}_{as}(\rho)$ and

$$\tilde{u}_{as}(\rho) = (e^{i\pi/2}\rho)^{-1/2+iq}e^{-i\rho/2} = e^{i(q\ln\rho-\rho/2-\pi/4+i\pi q/2)}\rho^{-1/2}, \tag{8.82}$$
$$u_{as}(x) = (c/2\upsilon)^{1/2}e^{i\{q[\ln(2\kappa/c)-cx]-(\upsilon/c)\exp(-cx)-\pi/4+i\pi q/2\}}e^{cx/2}, \tag{8.83}$$

i.e., any solution of (8.76) is square-integrable on $-\infty$ (for any W).

For $x \to \infty$ ($\rho \to 0$), we have

$$P(x;W) = \Gamma^{-1}(\beta)z^\mu\tilde{O}(\rho) = O\left(e^{-x|W|^{1/2}\sin(\varphi/2)}\right) \to 0,\ \operatorname{Im}W > 0,$$

and

$$u_1(x;W) = -\frac{\pi(2\kappa/c)^{-\mu}e^{-i\pi\mu/2}e^{-ix|W|^{1/2}\exp(\varphi/2)}}{\sin(2\pi\mu)\Gamma(\alpha_{-|+})\Gamma(\beta_-)}\tilde{O}(\rho)$$
$$= O\left(e^{x|W|^{1/2}\sin(\varphi/2)}\right) \to \infty,$$

for $0 < \operatorname{Im} W < b_0$, where

$$b_0 = \begin{cases} \min\left[c^2/2, g_2^2/(2\kappa^2)\right], \ g_2 \neq 0, \\ \infty, \ g_2 = 0. \end{cases}$$

Under such a limitation on W (which is enough for our aims), $\alpha_{\pm,\xi}, \beta_\pm \notin \mathbb{Z}_-$.

As far as

$$\mathrm{Wr}(u_1, u_2) = -ic\mathrm{e}^{-\pi q}, \ \mathrm{Wr}(u_1, P) = -c/\Gamma(\alpha), \ \mathrm{Wr}(u_2, P) = -c\mathrm{e}^{i\pi\mu}/\Gamma(\alpha_{+|-})$$

is concerned, both sets u_1, u_2 and u_1, P (the latter for $\operatorname{Im} W > 0$, $\alpha \notin \mathbb{Z}_-$) are fundamental sets of solutions of (8.76). Because $P(x; W) \in L^2(\mathbb{R})$ and $u_1(x; W) \notin L^2(\mathbb{R})$, there exists only one independent square-integrable solution of (8.76) for a fixed W ($\operatorname{Im} W > 0$) for all the values of parameters. This means that in the case under consideration, the deficiency indices of $\hat{H}$ are $m_\pm = 1$.

The adjoint $\hat{H}^+$ is defined on functions ψ_* from the natural domain $D^*_{\check{H}}(\mathbb{R})$. Such functions satisfy the equation

$$\check{H}\xi(x) = \eta(x) \in L^2(\mathbb{R}). \tag{8.84}$$

Regarding $V(x) \overset{x\to\infty}{\longrightarrow} 0$, we have $\psi_*(x), \psi_*'(x) \overset{x\to\infty}{\longrightarrow} 0$ (see Sect. 2.1), so that

$$\Delta_{H^+}(\psi_*) = -[\psi_*, \psi_*](-\infty), \ \forall\psi_* \in D^*_{\check{H}}(\mathbb{R}).$$

We can obtain the asymptotic behavior of ψ_* using the general solution

$$\begin{aligned}\psi_*(x) &= c_1u_1(x;0) + c_2u_2(x;0)\\ &\quad + ic^{-1}\mathrm{e}^{\pi q}\int_{-\infty}^{x}[u_1(x;0)u_2(y;0) - u_2(x;0)u_1(y;0)]\eta(y)\mathrm{d}y \end{aligned} \tag{8.85}$$

of (8.84).

To estimate integral terms on the right-hand side of (8.85), it is convenient to rewrite ψ_* and its derivative in terms of the variable ρ ($\tilde{\psi}_*(\rho) = \psi_*(x)$),

$$\begin{aligned}\tilde{\psi}_*(\rho) &= c_1\tilde{u}_1(\rho;0) + c_2\tilde{u}_2(\rho;0)\\ &\quad + ic^{-2}\mathrm{e}^{\pi q}\int_{\rho}^{\infty}[\tilde{u}_2(\rho;0)\tilde{u}_{+1}(\rho';0) - \tilde{u}_1(\rho;0)\tilde{u}_2(\rho';0)]\tilde{\eta}(\rho)\frac{\mathrm{d}\rho'}{\rho'},\\ \tilde{\psi}_*'(\rho) &= c_1 d_\rho\tilde{u}_1(\rho;0) + c_2 d_\rho\tilde{u}_2(\rho;0)\\ &\quad + ic^{-2}\mathrm{e}^{\pi q}\int_{\rho}^{\infty}[d_\rho\tilde{u}_2(\rho;0)\tilde{u}_1(\rho';0) - d_\rho\tilde{u}_1(\rho;0)\tilde{u}_2(\rho';0)]\tilde{\eta}(\rho)\frac{\mathrm{d}\rho'}{\rho'}.\end{aligned}$$

Using the fact that $\tilde{u}_1(\rho;0)$, $\tilde{u}_1'(\rho;0)$, $\tilde{u}_2(\rho;0)$, and $\tilde{u}_2'(\rho;0)$ have the asymptotics $O(\rho^{-1/2})$ as $\rho \to \infty$ $(x \to -\infty)$ and the Cauchy–Schwarz inequality, we obtain as $\rho \to \infty$,

$$\tilde{\psi}_*(\rho) = c_1\tilde{u}_{\mathrm{as}}(\rho) + c_2\overline{\tilde{u}_{\mathrm{as}}(\rho)} + O(\rho^{-1}),$$
$$\tilde{\psi}_*'(\rho) = c_1 d_\rho \tilde{u}_{\mathrm{as}}(\rho) + c_2\overline{d_\rho \tilde{u}_{\mathrm{as}}(\rho)} + O(\rho^{-2}),$$

where $\tilde{u}_{\mathrm{as}}(\rho)$ is defined by (8.82).

By the help of the asymptotics, we obtain $\Delta_{H^+}(\psi_*) = ic\mathrm{e}^{-\pi q}(\overline{c_1}c_1 - \overline{c_2}c_2)$, which confirms the fact that deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $c_1 = \exp(2i\theta)\, c_2$, $\theta \in \mathbb{S}(0,\pi)$.

Thus, in the range under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_\theta$ parameterized by $\theta \in \mathbb{S}(0,\pi)$ with domains D_{H_θ} that consist of functions belonging to $D^*_{\check{H}}(\mathbb{R})$ with the following asymptotic behavior as $x \to -\infty$:

$$\psi(x) = C\left[\mathrm{e}^{i\theta}u_{\mathrm{as}}(x) + \mathrm{e}^{-i\theta}\overline{u_{\mathrm{as}}(x)}\right] + O\left(\mathrm{e}^{-c|x|}\right), \tag{8.86}$$

where the function $u_{\mathrm{as}}(x)$ is defined by (8.83).

The general solution of (8.84) with $b_0 > \operatorname{Im} W > 0$, has the form

$$\psi(x) = c_1u_1(x;W) + c_2P(x;W) + c^{-1}\Gamma(\alpha)$$
$$\times\left[u_1(x;W)\int_x^\infty P(y;W)\eta(y)\mathrm{d}y + P(x;W)\int_{-\infty}^x u_1(y;W)\eta(y)\mathrm{d}y\right],$$

where $c_{1,2}$ are arbitrary constants. With the help of the Cauchy–Schwarz inequality, we can verify that both terms in square brackets are bounded as $x \to \infty$, which implies that for the function ψ to be square-integrable, the conditions $c_1 = 0$ must hold. Then we represent $\psi(x)$ as

$$\psi(x) = c_2P(x;W) + c^{-1}\Gamma(\alpha)\eta_P u_1(x;W) + c^{-1}\Gamma(\alpha)$$
$$\times\left[P(x;W)\int_{-\infty}^x u_1(y;W)\eta(y)\mathrm{d}y - u_1(x;W)\int_{-\infty}^x P(y;W)\eta(y)\mathrm{d}y\right],$$
$$\eta_P = \int_{-\infty}^\infty P(y;W)\eta(y)\mathrm{d}y. \tag{8.87}$$

Again, estimating integral terms in (8.87) with the help of the Cauchy–Schwarz inequality, we obtain as $x \to -\infty$,

$$\psi(x) = c_2 i\mathrm{e}^{\pi q}\left[\frac{\mathrm{e}^{i\pi\mu}u_{\mathrm{as}}(x)}{\Gamma(\alpha_{+|-})} - \frac{\overline{u_{\mathrm{as}}(x)}}{\Gamma(\alpha)}\right] + c^{-1}\Gamma(\alpha)\eta_P u_{\mathrm{as}}(x;W) + O\left(\mathrm{e}^{-c|x|}\right).$$

Then condition (8.86) implies

$$c_2 = ic^{-1}\Gamma(\alpha)\eta_P a_\theta^{-1}(\mu)\mathrm{e}^{-i\theta-\pi q}.$$

Using relations (8.80) and (8.81), we obtain the Green's function of the operator $\hat{H}_\theta$ from (8.87):

$$\begin{aligned} G(x, y; W) &= \Omega^{-1}(W)\, U_\theta(x, W)\, U_\theta(y; W) \\ &\quad - \frac{\mathrm{e}^{\pi q}}{2c}\begin{cases} \tilde{U}_\theta(x, W)\, U_\theta(y; W), & x > y, \\ U_\theta(x, W)\, \tilde{U}_\theta(y; W), & x < y, \end{cases} \\ \Omega(W) &= -i\,\frac{2ca_\theta(\mu)}{b_\theta(\mu)}\mathrm{e}^{-\pi q}\,. \end{aligned}$$

The imaginary part of the function $M(x_0, E+i0)$, given by (5.21), has the form

$$\begin{aligned} &\operatorname{Im} M(x_0, E+i0) = [U_\theta(x_0, E)]^2 \operatorname{Im} \Omega^{-1}(E+i0), \\ &\Omega(W) = -2ic\mathrm{e}^{-\pi q}\frac{\mathrm{e}^{i(\pi\mu/2-\theta)}\Gamma(1/2+\mu-iq) + \mathrm{e}^{-i(\pi\mu/2-\theta)}\Gamma(1/2+\mu+iq)}{\mathrm{e}^{i(\pi\mu/2-\theta)}\Gamma(1/2+\mu-iq) - \mathrm{e}^{-i(\pi\mu/2-\theta)}\Gamma(1/2+\mu+iq)}. \end{aligned}$$

Taking into account that $U_\theta(x, W)$ is a real entire function satisfying the boundary condition (8.86), one can prove that the guiding functional

$$\Phi(\xi; W) = \int_{\mathbb{R}} U_\theta(x, W)\, \xi(x)\mathrm{d}x,\ \xi \in \mathcal{D}_r(\mathbb{R}) \cap D_{H_\theta}$$

is simple, so that the spectra of the operators $\hat{H}_\theta$ are simple.

The derivative of the spectral function has the form $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E+i0)$. For $E = c^2p^2 \geq 0$, $p \geq 0$, $\mu = -ip$, we obtain

$$\sigma'(E) = \frac{\mathrm{e}^{\pi q}}{2\pi c}\frac{|D(E)|^2 - 1}{|D(E)+1|^2},\ D(E) = \frac{\Gamma(1/2 - ip - iq)}{\Gamma(1/2 - ip + iq)}\mathrm{e}^{-2i\theta+\pi p}.$$

A straightforward calculation gives

$$|D(E)| = \mathrm{e}^{\pi p}\sqrt{\frac{\cos h[\pi(p+q)]}{\cos h[\pi(p-q)]}} > 1,\ p > 0.$$

The derivative $\sigma'(E)$ is finite for $E \geq 0$ and θ satisfying the condition

$$\mathrm{e}^{2i\theta} \neq K = -\frac{\Gamma(1/2 - iq)}{\Gamma(1/2 + iq)}.$$

If $\mathrm{e}^{2i\theta} = K$, the derivative has an integrable singularity of the form $\sigma'(E) \sim E^{-1/2}$. Thus, any $E \in \mathbb{R}_+$ belongs to the continuous spectrum.

For $E = -c^2\tau^2 < 0$, $\tau > 0$, $\mu = \tau$, the function $\Omega(E)$ reads

$$\Omega(E) = -2c\mathrm{e}^{-\pi q}\cot[f(E) - \theta],$$
$$f(E) = \pi\tau/2 + \frac{1}{2i}\big[\ln\Gamma(1/2 + \tau - iq) - \ln\Gamma(1/2 + \tau + iq)\big]. \tag{8.88}$$

The function $\Omega^{-1}(E)$ is real at the points where $\Omega(E) \neq 0$. Thus, only the $E = E_n(\theta)$ obeying the equation

$$\Omega(E_n(\theta)) = 0 \Longrightarrow f(E_n(\theta)) = \pi/2 + \pi n + \theta,\ n \in \mathbb{Z}, \tag{8.89}$$

provide nonzero contributions to $\operatorname{Im}\Omega^{-1}(E + i0)$.

The derivative of the spectral function has the form

$$\sigma'(E) = \sum_{n\in\mathbb{Z}} Q_n^2\delta(E - E_n(\theta)),\ Q_n = \sqrt{\frac{\sqrt{|E_n(\theta|}\mathrm{e}^{\pi q}}{\pi/2 + \operatorname{Im}\psi(1/2 + c^{-1}\sqrt{|E_n(\theta|} - iq)}}.$$

Finally, we see that spec $\hat{H}_\theta$ equals $\mathbb{R}_+ \cup \{E_n(\theta),\ n \in \mathbb{Z}\}$ and is simple, the set of its (generalized) eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}U_\theta(x; E)$, $E \geq 0$, and $U_n(x) = Q_nU_\theta(x; E_n(\theta))$ form a complete orthonormalized system in $L^2(\mathbb{R})$.

Some remarks on the spectrum structure can be made: First of all, one can show that

$$f'(E) = -2\tau\,[\pi/2 + \operatorname{Im}\psi(1/2 + \tau - iq)] < 0,\ E < 0. \tag{8.90}$$

According to [81, 8.363.4], the expression $|\operatorname{Im}\psi(1/2 + \tau - iq)|$ is a monotonically decreasing function of τ for $\tau \geq 0$. For $\tau = 0$, we obtain [81, 8.365.9] that

$$|\operatorname{Im}\psi(1/2 - iq)| = \frac{\pi}{2}\tan h(\pi|q|) < \frac{\pi}{2} \Longrightarrow$$
$$\Longrightarrow |\operatorname{Im}\psi(1/2 + \tau - iq)| < \pi/2,$$

which implies (8.90). In addition, $f(E)$ has the properties

$$f(E) = \pi\tau/2 - q\ln\tau + O(1),\ E \to -\infty;$$
$$f(0) = -\zeta_q\phi_0 + O(\tau),\ \tau \to 0,$$
$$\phi_0 = \arctan(2|q|),\ \zeta_q = \operatorname{sgn} q = \operatorname{sgn} g_2,$$

and $\partial_\theta E_n = [f'(E_n(\theta))]^{-1} < 0$. Thus, as E passes from $-\infty$ to 0, the function $f(E)$ decreases monotonically from ∞ to $f(0) = -\zeta_q\phi_0$.

Because any number from the interval $R_f = (-\zeta_q\phi_0, \infty)$ can be represented as $\pi/2 + \pi(n + \theta/\pi)$ with some $n \geq -1$ and some $\theta \in (0, \pi]$, we have $n \in \{-1\} \cup \mathbb{Z}_+$, and any $E<0$ is a solution of (8.89) for some n and θ (depending, in general, on E).

Regarding $\partial_\theta E_n(\theta) < 0$ for a given $n \in \{-1\} \cup \mathbb{Z}_+$, we can draw the following conclusions: Let $\mathcal{E}_n$ be solutions of (8.89) for $n \in \mathbb{Z}_+$ and $\theta = 0$ (there exists only one solution for any fixed $n \in \mathbb{Z}_+$, and furthermore, $\mathcal{E}_{n+1} < \mathcal{E}_n$ for any n). Then in the interval $[\mathcal{E}_0, 0)$ there are no solutions of (8.89) for extensions with $\theta \in (0, \theta_0 = \pi/2 - \zeta_q\phi_0]$, and for any fixed $\theta \in (\theta_0, \pi]$, there is one solution $E_{-1}(\theta)$ monotonically decreasing from -0 to $E_{-1}(\pi) = \mathcal{E}_0$ as θ goes from $\theta_0 + 0$ to π; in any interval $[\mathcal{E}_{n+1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, for a fixed $\theta \in (0, \pi]$, there is one solution $E_n(\theta)$ monotonically decreasing from $\mathcal{E}_n - 0$ to $\mathcal{E}_{n+1}$ as θ goes from $+0$ to π. We stress that the relations

$$E_{n-1}(\pi) = \lim_{\theta \to 0} E_n(\theta) = E_n(0) = \mathcal{E}_n,\ n \in \mathbb{Z}_+$$

confirm once again the equivalence of extensions $\theta = \pi$ and $\theta = 0$.

8.5.3 *Range 3*

In this range, we have $g_1 = 0$. Below, we list briefly only the principal results.

8.5.3.1 Subrange $g_2 = \upsilon^2 > 0, \upsilon > 0$

In this subrange, it is convenient to introduce a new variable ζ,

$$\zeta = 2\upsilon c^{-1} \mathrm{e}^{-cx/2},\ x = -\ln(cz/2\upsilon),\ dx = -dz/cz,\ z \in \mathbb{R}_+,$$

and a new function $\phi(\zeta) = \psi(x)$ to transform (8.76) to the Bessel equation of the imaginary argument,

$$\left[d_\zeta^2 + \zeta^{-1} d_\zeta - (1 + \zeta^{-2} 4\mu^2)\right] \phi(\zeta) = 0,\ \mu = c^{-1}\sqrt{-W}.$$

One can see that the deficiency indices of $\hat{H}$ are $m_\pm = 0$, so that there exists only one s.a. Hamiltonian $\hat{H}_1 = \hat{H}^+$.

One can verify that the guiding functional (8.78) with $u_1(x; W) = K_{2\mu}(\zeta)$, where $K_{2\mu}(\zeta)$ is a real entire solution of (8.76), is simple, and therefore the spectrum of $\hat{H}_1$ is simple.

One can see that for $E = c^2 p^2 \geq 0,\ p \geq 0$, we have

$$\sigma'(E) = \frac{2\theta(E)}{\pi^2 c} \sin h\,(2\pi p),$$

so that the simple spectrum of $\hat{H}_1$ reads spec $\hat{H}_1 = \mathbb{R}_+$, and the generalized eigenfunctions

$$U_E(x) = \sqrt{\frac{2\sin h\,(2\pi p)}{\pi^2 c}} K_{2ip}(\zeta)$$

of $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R})$.

8.5.3.2 Subrange $g_2 = -\upsilon^2 < 0$, $\upsilon > 0$

Introducing $\zeta = c^{-1}\upsilon e^{-cx/2}$ and the function $f(\zeta) = \psi(x)$, we transform (8.76) to the Bessel equation

$$\left[d_\zeta^2 + \zeta^{-1}d_\zeta + \left(1 - \zeta^{-2}(2\mu)^2\right)\right] f(\zeta) = 0,\ \mu = c^{-1}\sqrt{-W}.$$

Deficiency indices of $\hat{H}$ are $m_\pm = 1$, and there exists a family of s.a. extensions $\hat{H}_\theta$, parameterized by $\theta \in \mathbb{S}(0,\pi)$, with domains D_{H_θ} that consist of functions from $D^*_{\check{H}}(\mathbb{R})$ with the following asymptotic behavior as $x \to -\infty$:

$$\psi(x) = C\left[e^{i\theta}v_{as}(x) + e^{-i\theta}\overline{v_{as}(x)}\right] + O\left(e^{-3c|x|/4}\right),$$
$$v_{as}(x) = e^{-i[(2\upsilon/c)e^{-cx/2} + \pi/4]}e^{cx/4}. \quad (8.91)$$

One can verify that the guiding functional (8.78) with $u_1(x;W) = U_\theta(x;W)$, where

$$U_\theta(x;W) = \frac{\sqrt{\pi}}{2}\left[e^{i(\theta-\pi\mu-1/2)}H_{2\mu}^{(2)}(\zeta) + e^{-i(\theta-\pi\mu-1/2)}H_{2\mu}^{(1)}(\zeta)\right],$$

is a real entire solution of (8.76) satisfying s.a. boundary condition (8.91). Also, it is simple, and therefore the spectra of $\hat{H}_\theta$ are simple.

For $E = c^2p^2 \geq 0$, $p \geq 0$, we have

$$\sigma'(E) = \frac{(\pi c)^{-1}\sin h(2\pi p)}{\cos(2\theta) + \cos h(2\pi p)}.$$

For $E = -c^2\tau^2 < 0$, $\tau > 0$, we have

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\theta)),\ Q_n = \left(2\sqrt{|E_n(\theta)|}/\pi\right)^{1/2},$$

where

$$E_n(\theta) = -c^2(1 + 2\pi^{-1}\theta + 2n)^2,$$
$$n \in \begin{cases} \{-1\} \cup \mathbb{Z}_+, & \pi/2 < \theta \leq \pi, \\ \mathbb{Z}_+, & 0 \leq \theta \leq \pi/2, \end{cases}$$
$$E_{n-1}(\pi) = E_n(0),\ n \in \mathbb{Z}_+.$$

Finally, the simple spectrum of $\hat{H}_\theta$ is given by spec $\hat{H}_\theta = \mathbb{R}_+ \cup \{E_n(\theta)\}$. The (generalized) eigenfunctions $U_E(x) = \sqrt{\sigma'(E)}U_\theta(x; E)$, $E \geq 0$, and $U_n(x) = Q_n U_\theta(x; E_n(\theta))$ of $\hat{H}_\theta$ form a complete orthonormalized system in $L^2(\mathbb{R})$.

We note that all the results in the case $g_1 = 0$ under consideration can be derived from the corresponding results obtained for $g_1 \neq 0$. To see this, we first set $g_2 = 0$, and then perform the following change of notation: $g_1, c, \mu, p, \tau \to \tilde{g}_1, \tilde{c}, \tilde{\mu}, \tilde{p}, \tilde{\tau}$. In the new notation,

$$\tilde{\mu} = \tilde{c}^{-1}\sqrt{-W},\ E = \begin{cases} \tilde{c}^2\tilde{p}^2,\ E \geq 0, \\ -\tilde{c}^2\tilde{\tau}^2,\ E < 0. \end{cases}$$

In addition, one needs to make the change $\tilde{g}_1 = g_2$, $\tilde{c} = c/2$, $\tilde{\mu} = 2\mu$, $\tilde{p} = 2p$, and $\tilde{\tau} = 2\tau$ in all the expressions to arrive at the case $g_1 = 0$. Then expressions that arise are simplified. For example,

$$\begin{aligned} P(x; W) &= \Gamma^{-1}(\beta)z^\mu e^{-z/2}\Phi(\alpha, \beta; z) \to P(x; W) = \Gamma^{-1}(\beta)z^\mu e^{-z/2}\Phi(\beta/2, \beta; z) \\ &= \frac{4^\mu \Gamma(1+\mu)}{\Gamma(1+2\mu)} I_\mu(z/2), \\ u_1(x; W) &= z^\mu e^{-z/2}\Psi(\alpha, \beta; z) \to u_1(x; W) \\ &= z^\mu e^{-z/2}\Psi(\beta/2, \beta; z) = \pi^{-1/2}K_\mu(z/2) \end{aligned}$$

(see [1, 20, 81]), so that expression (8.88) and (8.89) take the form

$$\Omega(E) = \cot\left[f(E) - \theta\right],\ \ f(E) = \pi\tau/2,\ \ \pi\tau_n/2 - \theta = \pi/2 + \pi n.$$

8.6 ESP VI

In this case,

$$V(x) = c^2 g_1 \sin^{-2}(cx) + c^2 g_2 \cos^{-2}(cx),\ \ x \in [0, \pi/2c], \tag{8.92}$$

and the corresponding Schrödinger equation is

$$\psi'' - c^2[g_1 \sin^{-2}(cx) + c^2 g_2 \cos^{-2}(cx)]\psi + W\psi = 0. \tag{8.93}$$

It is sufficient to consider only the case $c > 0$ without loss of generality. The potential (8.92) is known as *the Pöschl–Teller potential*; see [126]. This potential was used to study the vibron model of a molecular system and describe anharmonic effects in the dissociation [105].

Introducing a new variable z and new functions $\phi_{\xi_\mu}(z)$, instead of x and $\psi(x)$ in (8.93),

$$z = \sin^2(cx),\ z \in [0,1],$$
$$\psi(x) = z^{1/4+\xi_\mu \mu/2}(1-z)^{1/4+\nu/2}\phi_{\xi_\mu}(z),\ \xi_\mu = \pm 1,$$

where

$$\mu = \begin{cases} \sqrt{g_1 + 1/4},\ g_1 \geq -1/4, \\ i\varkappa,\ \varkappa = \sqrt{|g_1| - 1/4},\ g_1 < -1/4, \end{cases} \quad \mu^2 = g_1 + 1/4;$$

$$\nu = \begin{cases} \sqrt{g_2 + 1/4},\ g_2 \geq -1/4, \\ i\kappa,\ \kappa = \sqrt{|g_2| - 1/4},\ g_2 < -1/4, \end{cases} \quad \nu^2 = g_2 + 1/4,$$

we obtain equations for the new functions,

$$\begin{aligned} &z(1-z)d_z^2\phi_{\xi_\mu}(z) + [\gamma_{\xi_\mu} - (1 + \alpha_{\xi_\mu} + \beta_{\xi_\mu})z]d_z\phi_{\xi_\mu}(z) - \alpha_{\xi_\mu}\beta_{\xi_\mu}\phi_{\xi_\mu}(z) = 0\ , \\ &\alpha_{\xi_\mu} = (1 + \xi_\mu\mu + \nu + \lambda)/2,\ \beta_{\xi_\mu} = (1 + \xi_\mu\mu + \nu - \lambda)/2,\ \gamma_{\xi_\mu} = 1 + \xi_\mu\mu, \\ &w = W/c^2 = |w|e^{i\varphi},\ 0 \leq \varphi < 2\pi,\ \lambda = \sqrt{|w|}e^{i\varphi/2}. \end{aligned} \tag{8.94}$$

Introducing a new variable u and a new function $\phi(u)$ instead of x and $\psi(x)$ in (8.93),

$$u = 1 - z,\ \psi(x) = (1-u)^{1/4+\mu/2}u^{1/4+\nu/2}\phi(u),$$

we obtain an equation for $\phi(u)$,

$$\begin{aligned} &u(1-u)d_u^2\phi(u) + [\gamma' - (1 + \alpha' + \beta')u]d_u\phi(u) - \alpha'\beta'\phi(u) = 0, \\ &\alpha' = (1 + \mu + \nu + \lambda)/2,\ \beta' = (1 + \mu + \nu - \lambda)/2,\ \gamma' = 1 + \nu. \end{aligned} \tag{8.95}$$

Equations (8.94) and (8.95) have hypergeometric functions $F(\alpha, \beta; \gamma; z)$ as solutions; see [20, 81]. Using these functions, we can construct solutions of (8.93).

We use three solutions of (8.93) in what follows:

$$\begin{aligned} u_1(x;W) &= z^{1/4+\mu/2}(1-z)^{1/4+\nu/2}F(\alpha_1, \beta_1; \gamma_1; z) = u_1(x;W)|_{\nu\to-\nu}, \\ u_2(x;W) &= z^{1/4-\mu/2}(1-z)^{1/4+\nu/2}F(\alpha_2, \beta_2; \gamma_2; z) = u_2(x;W)|_{\nu\to-\nu}, \\ V_1(x;W) &= z^{1/4+\mu/2}(1-z)^{1/4+\nu/2}F(\alpha_1, \beta_1; \gamma_3; 1-z) = V_1(x;W)|_{\mu\to-\mu}, \end{aligned}$$

where

$$\begin{aligned} &\alpha_1 = (1 + \mu + \nu + \lambda)/2,\ \beta_1 = (1 + \mu + \nu - \lambda)/2, \\ &\alpha_2 = (1 - \mu + \nu + \lambda)/2,\ \beta_2 = (1 - \mu + \nu - \lambda)/2, \\ &\gamma_1 = 1 + \mu,\ \gamma_2 = 1 - \mu,\ \gamma_3 = 1 + \nu. \end{aligned}$$

We note that $u_2(x;W) = u_1(x;W)|_{\mu\to-\mu}$. There is a relation between these solutions:

$$V_1 = \frac{\Gamma(\gamma_3)\Gamma(-\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}u_1 + \frac{\Gamma(\gamma_3)\Gamma(\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_2.$$

We note that the functions $u_k(x;W)$, $k = 1, 2$, are entire in W for any g_1 and g_2. They are real entire in W for $g_1 \geq -1/4$ ($\mu \geq 0$), and $u_2(x;E) = \overline{u_1(x;E)}$ for $g_1 < -1/4$ ($\mu = i\varkappa$). The function $V_1(x;W)$ is entire in W and real entire in W for $g_2 \geq -1/4$ ($\nu \geq 0$).

8.6.1 Range 1

In this range, we have

$$g_2 \geq 3/4 \ (\nu \geq 1)\,.$$

The asymptotic behavior of special functions in solutions (8.95) are well known, see [1, 20, 81], so that we can find their asymptotics.

As $x \to 0$, we have

$$u_1(x;W) = u_{1\mathrm{as}}(x)\tilde{O}(x^2),\ u_{1\mathrm{as}}(x) = (cx)^{1/2+\mu}, \tag{8.96}$$

$$u_2(x;W) = u_{2\mathrm{as}}(x)\tilde{O}(x^2),\ u_{2\mathrm{as}}(x) = (cx)^{1/2-\mu},$$

$$V_1(x;W) = \begin{cases} \frac{\Gamma(\gamma_3)\Gamma(\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_{2\mathrm{as}}(x)\tilde{O}(x^2),\ \mu \geq 1,\ g_1 \geq 3/4, \\ \left[\frac{\Gamma(\gamma_3)\Gamma(-\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}u_{1\mathrm{as}} + \frac{\Gamma(\gamma_3)\Gamma(\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_{2\mathrm{as}}(x)\right]\tilde{O}(x^2), \\ g_1 < 3/4,\ g_1 \neq -1/4. \end{cases} \tag{8.97}$$

As $x \to \pi/2c$, $v = \pi/2c - x \to 0$, we have

$$V_1(x;W) = (cv)^{1/2+\nu}\tilde{O}(v^2),\ \mathrm{Im}\,W > 0,$$

$$u_1(x;W) = \frac{\Gamma(\gamma_1)\Gamma(\nu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}(cv)^{1/2-\nu}\tilde{O}(v^2),\ \mathrm{Im}\,W > 0 \text{ or } W = 0.$$

The above asymptotics allow us to obtain

$$\mathrm{Wr}(u_1, u_2) = -2\mu c,\ \mathrm{Wr}(u_1, V_1) = -\frac{2c\Gamma(\gamma_1)\Gamma(\gamma_3)}{\Gamma(\alpha_1)\Gamma(\beta_1)} = -\omega(W).$$

It is easily seen that

$$\psi_* \in D^*_{\check{H}}(0, \pi/2c) \Longrightarrow \psi_*, \check{H}\psi_* \in L^2(0, \pi/4c) \Longrightarrow \psi_* \in D^*_{\check{H}}(0, \pi/4c).$$

Representing the potential (8.92) as $V(x) = g_1 x^{-2} + v(x)$, where $v(x)$ is a bounded function on $[0, \pi/4c]$, we can treat $\psi_*(x)$ on the interval $(0, \pi/4c]$ as a solution of the equation

$$-\psi_*''(x) + g_1 x^{-2}\psi_*(x) = \eta(x),\ \eta(x) = \check{H}\psi_*(x) - v(x)\psi_*(x) \in L^2(0, \pi/4c).$$

Asymptotic behavior of such functions as $x \to 0$ was studied in Sect. 7.2, so that we have

$$\psi_*(x) = \psi_*^{\text{as}}(x) + \begin{cases} O(x^{3/2}),\ g_1 \neq 3/4, \\ O\left(x^{3/2}\sqrt{\ln x}\right),\ g_1 = 3/4, \end{cases}$$

$$\psi_*'(x) = \psi_*^{\text{as}\prime}(x) + \begin{cases} O(x^{1/2}),\ g_1 \neq 3/4, \\ O\left(x^{1/2}\sqrt{\ln x}\right),\ g_1 = 3/4, \end{cases}$$

where

$$\psi_*^{\text{as}}(x) = \begin{cases} 0,\ g_1 \geq 3/4, \\ c_1\,(k_0 x)^{1/2+\mu} + c_2\,(k_0 x)^{1/2-\mu},\ g_1 < 3/4,\ g_1 \neq -1/4, \\ c_1 x^{1/2} + c_2 x^{1/2}\ln(k_0 x),\ g_1 = -1/4. \end{cases}$$

8.6.1.1 Subrange $g_2 \geq 3/4$, $g_1 \geq 3/4$

We note that for $g_1 \geq 3/4$ ($\mu \geq 1$), the solution $V_1(x; W)$ is not square-integrable at the origin, but for $g_1 < 3/4$, it is (moreover, any solution is square-integrable at the origin). This means that for $g_1 \geq 3/4$, (8.93) has no square-integrable solutions, and the deficiency indices of the initial symmetric Hamiltonian $\hat{H}$ are zero. This implies that the operator $\hat{H}^+$ is s.a. and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$ with domain $D_{H_1} = D^*_{\check{H}}(0, \pi/2c)$.

The general solution of inhomogeneous equation

$$\left(\check{H} - W\right)\psi = \eta \in L^2\,(0, \pi/2c)\,,\ \operatorname{Im} W > 0,$$

can be represented as

$$\psi(x) = a_1 u_1(x; W) + a_2 V_1(x; W) + I(x; W),\ I(x; W) = \omega^{-1}(W)$$
$$\times\left[u_1(x; W)\int_x^{\pi/2c} V_1(y; W)\eta(y)\mathrm{d}y + V_1(x; W)\int_0^x u_1(y; W)\eta(y)\mathrm{d}y\right]. \tag{8.98}$$

Using the Cauchy–Schwarz inequality, we estimate that $I(x) = O((\pi/2c - x)^{3/2})$ as $x \to \pi/2c$ (with logarithmic accuracy for $g_2 = 3/4$). The condition $\psi_* \in L^2(0, \pi/2c)$ implies $a_1 = 0$ for any g_1. Similarly, we obtain $I(x) = O(x^{3/2})$ as $x \to 0$ (with logarithmic accuracy for $g_1 = 3/4$) and the condition $\psi_* \in L^2(0, \pi/2c)$ implies $a_2 = 0$.

Thus, the Green's function of the operator $\hat{H}_1$ has the form

$$G(x, y; W) = \omega^{-1}(W) \begin{cases} V_1(x; W)u_1(y; W), & x > y, \\ u_1(x; W)V_1(y; W), & x < y, \end{cases}$$

so that

$$M(x_0; W) = G(x_0 - 0, x_0 + 0; W) = \omega^{-1}(W)u_1(x_0; W)V_1(x_0; W).$$

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^{\pi/2c} u_1(x; W)\xi(x)\mathrm{d}x, \ \xi \in D_r(0, \pi/2c) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ ($\tilde{U} = V_1$), and therefore the spectrum of $\hat{H}_1$ is simple.

Following Chap. 5, we obtain the derivative of the spectral function,

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega^{-1}(E + i0), \ \ \Omega(W) = \omega(W)\frac{u_1(x_0; W)}{V_1(x_0; W)}.$$

Let $E = -c^2\tau^2 \le 0$, $\tau \ge 0$, $\lambda = i\tau$. In this case all the quantities $u_1(x_0; E)$, $V_1(x_0; E)$, and $\omega(E)$ are real and finite, and $\omega(E) \neq 0$, so that $\sigma'(E) = 0$.

Let $E = c^2p^2 > 0$, $p > 0$, $\lambda = p$. In this case $\Omega^{-1}(E)$ is real except for the energies where $\Omega(E) = \infty$. The latter is possible only for $\beta_1 = -n$, $n \in \mathbb{Z}_+$. Therefore, in this case,

$$\sigma'(E) = \frac{1}{2\pi c} \left.\frac{V_1(x_0; E)\Gamma(\alpha_1)}{u_1(x_0; E)\Gamma(\gamma_1)\Gamma(\gamma_3)}\right|_{W=E} \operatorname{Im} \Gamma(\beta_1)|_{W=E+i0}\,.$$

Near the points $\beta_1 = -n$ or $1 + \mu + \nu - \lambda_n = -2n$, we obtain (using Lemma 5.17)

$$\begin{aligned}
&W = E - E_n + i\varepsilon, \ \beta_1 = -n - \frac{E - E_n + i\varepsilon}{4c^2 p_n}, \\
&\operatorname{Im} \Gamma(\beta_1)|_{W=E+i0} = (-1)^n \frac{4\pi c^2 p_n}{n!}\delta(E - E_n), \\
&\lambda_n = p_n = 1 + \mu + \nu + 2n, \ E_n = c^2(1 + \mu + \nu + 2n)^2, \qquad (8.99) \\
&V_1(x_0; E_n) = (-1)^n \frac{\Gamma(\gamma_3)\Gamma(1 + \mu + n)}{\Gamma(\gamma_3 + n)\Gamma(\gamma_1)} u_1(x_0; E_n),
\end{aligned}$$

and

$$\sigma'(E) = \sum_{n=0}^{\infty} Q_n^2 \delta(E - E_n), \ Q_n = \sqrt{\frac{2cp_n}{n!} \frac{\Gamma(\gamma_1 + \nu + n)\Gamma(\gamma_1 + n)}{\Gamma^2(\gamma_1)\Gamma(\gamma_3 + n)}}. \tag{8.100}$$

Finally, we obtain that the simple spectrum of $\hat{H}_1$ reads spec $\hat{H}_1 = \{E_n, \ n \in \mathbb{Z}_+\}$. The eigenfunctions $U_n(x) = Q_n u_1(x; E_n)$, $n \in \mathbb{Z}_+$, form a complete orthonormalized system in $L^2(0, \pi/2c)$.

8.6.1.2 Subrange $g_2 \geq 3/4, 3/4 > g_1 > -1/4, \ 1 > \mu > 0$

In this subrange, we have as $x \to 0$,

$$\begin{aligned} \psi_*(x) &= a_1 u_{1\mathrm{as}}(x) + a_2 u_{2\mathrm{as}}(x) + O\left(x^{3/2}\right), \\ \psi_*'(x) &= a_1 u_{1\mathrm{as}}'(x) + a_2 u_{2\mathrm{as}}'(x) + O\left(x^{1/2}\right). \end{aligned} \tag{8.101}$$

Using the asymptotics of functions $u_1(x; W)$ and $V_1(x; W)$, one can verify that $[\psi_*, \psi_*](\pi/2c) = 0$. Using (8.101), we obtain $\Delta_{H^+}(\psi_*) = -2\mu c(\overline{a_1}a_2 - \overline{a_2}a_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies

$$a_1 \cos\zeta = a_2 \sin\zeta, \ \ \zeta \in \mathbb{S}(-\pi/2, \pi/2).$$

Thus, in the range under consideration, there exists a family of s.a. Hamiltonians $\hat{H}_{2,\zeta}$ parameterized by ζ with domains $D_{H_{2,\zeta}}$ that consist of functions from $D^*_{\check{H}}(0, \pi/2c)$ with the following asymptotic behavior as $x \to 0$:

$$\begin{aligned} &\psi(x) = C\psi_{2,\zeta\mathrm{as}}(x) + O\left(x^{3/2}\right), \ \psi'(x) = C\psi_{2,\zeta\mathrm{as}}'(x) + O\left(x^{1/2}\right), \\ &\psi_{2,\zeta\mathrm{as}}(x) = u_{1\mathrm{as}}(x)\sin\zeta + u_{2\mathrm{as}}(x)\cos\zeta. \end{aligned} \tag{8.102}$$

Therefore,

$$D_{H_{2,\zeta}} = \left\{\psi \in D^*_{\check{H}}(0, \pi/2c), \ \psi \text{ satisfy } (8.102)\right\}.$$

To obtain Green's functions of the operators $\hat{H}_{2,\zeta}$, we impose boundary condition (8.102) on the functions (8.98) (with $a_1 = 0$). Using asymptotics (8.96) and (8.97), we obtain the coefficient a_2 and then, following Sect. 5.3.2, the Green's functions

$$\begin{aligned} G(x, y; W) = &\ \Omega^{-1}(W)U_{2,\zeta}(x; W)U_{2,\zeta}(y; W) \\ &- \frac{1}{2\mu c}\begin{cases} \tilde{U}_{2,\zeta}(x; W)U_{2,\zeta}(y; W), \ x > y, \\ U_{2,\zeta}(x; W)\tilde{U}_{2,\zeta}(y; W), \ x < y. \end{cases} \end{aligned} \tag{8.103}$$

Here

$$U_{2,\zeta}(x;W) = u_1(x;W)\sin\zeta + u_2(x;W)\cos\zeta,$$

$$\tilde{U}_{2,\zeta}(x;W) = u_1(x;W)\cos\zeta - u_2(x;W)\sin\zeta,$$

$$\Omega(W) = -2\mu c\frac{\omega_{2,\zeta}(W)}{\tilde{\omega}_{2,\zeta}(W)},\ \omega_{2,\zeta}(W) = f(W)\cos\zeta - \sin\zeta,$$

$$\tilde{\omega}_{2,\zeta}(W) = f(W)\sin\zeta + \cos\zeta,\ f(W) = \frac{\Gamma(-\mu)\Gamma(\alpha_1)\Gamma(\beta_1)}{\Gamma(\mu)\Gamma(\alpha_2)\Gamma(\beta_2)},$$

and we used the relation

$$2\mu c V_1 = \omega(W)\left[\tilde{\omega}_{2,\zeta}(W)U_{2,\zeta} + \omega_{2,\zeta}(W)\tilde{U}_{2,\zeta}\right].$$

The second summand on the right-hand side of (8.103) is real for real $W = E$. We note that both $U_{2,\zeta}$ and $\tilde{U}_{2,\zeta}$ are solutions of (8.93) real entire in W, and the solutions $U_{2,\zeta}$ satisfy the boundary condition (8.102).

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^{\pi/2c} U_{2,\zeta}(x;W)\xi(x)\mathrm{d}x,\ \xi\in D_r(0,\pi/2c)\cap D_{H_{2,\zeta}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{2,\zeta}$ ($\tilde{U} = \tilde{U}_{2,\zeta}$), and therefore the spectra of $\hat{H}_{2,\zeta}$ are simple.

The derivative of the spectral function reads $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E+i0)$. The function $\Omega^{-1}(E)$ is real for any E where $\Omega(E)\neq 0$. That is why only the points $E_n(\zeta)$ obeying the equation $\Omega(E_n(\zeta)) = 0$ can provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta(E - E_n(\zeta)),\ Q_n = \sqrt{-\left[\Omega'(E_n(\zeta))\right]^{-1}},$$

where $\Omega'(E_n(\zeta)) < 0$.

Let us consider the extension with $\zeta = \pi/2$. Here $U_{2,\pi/2}(x;W) = u_1(x;W)$ and

$$\sigma'(E) = -\left.\frac{(2\pi\mu c)^{-1}\Gamma(\gamma_2)\Gamma(\alpha_1)}{\Gamma(\gamma_1)\Gamma(\alpha_2)\Gamma(\beta_2)}\right|_{W=E}\operatorname{Im}\Gamma(\beta_1)|_{W=E+i0}.$$

One can see that in this case the spectrum and inversion formulas can be derived from results obtained in the previous subrange. Namely, here $\sigma'(E) = \sum_{n\in\mathbb{Z}_+} Q_n^2\delta(E - \mathcal{E}_n)$, where $\mathcal{E}_n$ and Q_n are given by expressions for E_n and Q_n in (8.99) and (8.100) respectively.

The same results hold for the extension with $\zeta = -\pi/2$.

For the extension with $\zeta = 0$, we have $U_{2,0}(x;W) = u_2(x;W)$ and $\sigma'(E) = \sum_{n\in\mathbb{Z}_+} Q_n^2 \delta(E - E_n(0))$, where $E_n(0)$ are determined by the equation $\beta_2 = -n$, so that

$$E_n(0) = c^2(1 - \mu + \nu + 2n)^2 > 0,\ n \in \mathbb{Z}_+,$$

and the coefficients Q_n read

$$Q_n = \sqrt{\frac{2c\,(1 - \mu + \nu + 2n)\,\Gamma(\gamma_2 + \nu + n)\Gamma(\gamma_2 + n)}{n!\Gamma^2(\gamma_2)\Gamma(\gamma_3 + n)}}.$$

We note that $E_n(0) < \mathcal{E}_n < E_{n+1}(0) < \mathcal{E}_{n+1}$.

All these results coincide with those for the region $g_1 \geq 3/4$ if we substitute μ by $-\mu$.

For the extensions with $|\zeta| < \pi/2$, we can represent $\sigma'(E)$ and the spectrum equation as

$$\sigma'(E) = \sum_{n\geq n_{\min}} Q_{\zeta|n}^2 \delta(E - E_n(\zeta)),\ Q_{\zeta|n} = \sqrt{\left[2\mu c f_\zeta'(E_n(\zeta))\right]^{-1}},$$
$$f(E_n(\zeta)) = \tan\zeta,\ f_\zeta(W) = f(W) - \tan\zeta,\ f'(E_n(\zeta)) > 0.$$

We note that

$$f(E) \overset{E\to-\infty}{\longrightarrow} -\infty,\ f(\mathcal{E}_n \pm 0) = \mp\infty,\ \partial_\zeta E_n(\zeta) = \left[f'(E_n(\zeta))\cos^2\zeta\right]^{-1} > 0.$$

Then one can see that for any $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, there exists one discrete level $E_n(\zeta)$ monotonically increasing from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ as ζ goes from $-\pi/2 + 0$ to $\pi/2 - 0$ (we set $\mathcal{E}_{-1} = -\infty$). Furthermore, we find that $n_{\min} = 0$.

Thus, the simple spectra of operators $\hat{H}_{2,\zeta}$ read spec $\hat{H}_{2,\zeta} = \{E_n(\zeta),\ n \in \mathbb{Z}_+\}$. The eigenfunctions $U_n(x) = Q_{\zeta|n} U_{2,\zeta}(x; E_n(\zeta))$ of the Hamiltonian $\hat{H}_{2,\zeta}$ form a complete orthonormalized system in $L^2(0, \pi/2c)$.

8.6.1.3 Subrange $g_2 \geq 3/4$, $g_1 = -1/4$, $\mu = 0$

In this subrange the solutions $u_1(x;W)$ and $u_2(x;W)$ are dependent ($u_1 = u_2$), so that we are going to use solutions $u_1(x;W)$, $u_3(x;W)$, and $V_1(x;W)$ that are real entire in W,

$$
\begin{aligned}
&u_1(x;W) = z^{1/4}(1-z)^{1/4+\nu/2}F(\alpha,\beta;1;z),\ u_3(x;W) \\
&\qquad = \frac{\partial}{\partial\mu}z^{1/4+\mu/2}(1-z)^{1/4+\nu/2}F(\alpha_1,\beta_1;\gamma_1;z)\Big|_{\mu=0} = u_3(x;W)|_{\nu\to-\nu}, \\
&V_1(x;W) = z^{1/4}(1-z)^{1/4+\nu/2}F(\alpha,\beta;\gamma;1-z), \\
&\alpha=\alpha_+,\ \alpha_\pm=(1\pm\nu+\lambda)/2,\ \beta=\beta_+,\ \beta_\pm=(1\pm\nu-\lambda)/2,\ \gamma=1+\nu.
\end{aligned}
$$

There is a relation between these solutions:

$$
\begin{aligned}
V_1(x;W) &= j(W)\,\Gamma(\gamma)u_1(x;W) - \frac{2\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}u_3(x;W), \\
j(W) &= \frac{\partial}{\partial\mu}\frac{2\Gamma(\gamma_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)}\Big|_{\mu=0} = -\frac{2\mathbf{C}+\psi(\alpha)+\psi(\beta)}{\Gamma(\alpha)\Gamma(\beta)}.
\end{aligned}
$$

As $x\to 0$ or $x\to\pi/2c$ the above solutions have the following asymptotic behavior: As $x\to 0$, $z=(cx)^2\tilde{O}(x^2)\to 0$, we have

$$
\begin{aligned}
&u_1(x;W) = u_{1\mathrm{as}}(x)\tilde{O}(x^2),\ u_{1\mathrm{as}}(x) = (cx)^{1/2}, \\
&u_3(x;W) = u_{3\mathrm{as}}(x;W)\tilde{O}(x^2),\ u_{3\mathrm{as}}(x;W) = (cx)^{1/2}\ln(cx), \\
&V_1(x;W) = (cx)^{1/2}\left[j(W)\,\Gamma(\gamma) - \frac{2\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\ln(cx)\right]\tilde{O}(x^2\ln x).
\end{aligned}
\tag{8.104}
$$

As $x\to\pi/2c$, $1-z=(cy)^2\tilde{O}(y^2)\to 0$, $z\to 1$, $y=\pi/2c-x$, $\operatorname{Im}W>0$, we have

$$
\begin{aligned}
u_1(x;W) &= \frac{\Gamma(\nu)}{\Gamma(\alpha)\Gamma(\beta)}(cy)^{1/2-\nu}\tilde{O}(y^2), \\
V_1(x;W) &= (cy)^{1/2+\nu}\tilde{O}(y^2).
\end{aligned}
$$

Using the above asymptotics, we obtain

$$
\mathrm{Wr}(u_1,u_3) = c,\ \mathrm{Wr}(u_1,V_1) = -\frac{2c\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} = -\omega(W).
$$

The solutions u_1 and V_1 form a fundamental set of solutions of (8.93) for $\operatorname{Im}W\neq 0$ and $W=0$.

As was established at the beginning of this section, the functions $\psi_*\in D_{\check{H}}^*(0,\pi/2c)$ have the following asymptotics:

$$
\begin{aligned}
\psi_*(x) &= a_1u_{1\mathrm{as}}(x) + a_2u_{3\mathrm{as}}(x) + O(x^{3/2}), \\
\psi_*'(x) &= a_1u_{1\mathrm{as}}'(x) + a_2u_{3\mathrm{as}}'(x) + O(x^{1/2}),
\end{aligned}
$$

as $x \to 0$, and $[\chi_*, \psi_*](\pi/2c) = 0$. Using these results, we obtain $\Delta_{H^+}(\psi_*) = c(\overline{a_1}a_2 - \overline{a_2}a_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies

$$a_1 \cos\vartheta = a_2 \sin\vartheta,\ \vartheta \in \mathbb{S}(-\pi/2, \pi/2).$$

Thus, in the subrange under consideration, there exists a family of s.a. $\hat{H}_{3,\vartheta}$ parameterized by ϑ with domains $D_{H_{3,\vartheta}}$ that consist of functions from $D^*_{\check{H}}(0, \pi/2c)$ with the following asymptotic behavior as $x \to 0$:

$$\begin{aligned}
\psi(x) &= C\psi_{3,\vartheta\,\mathrm{as}}(x) + O(x^{3/2}\ln x),\\
\psi'(x) &= C\psi'_{3,\vartheta\,\mathrm{as}}(x) + O(x^{1/2}\ln x),\\
\psi_{3,\vartheta\,\mathrm{as}}(x) &= u_{1\mathrm{as}}(x)\sin\vartheta + u_{3\mathrm{as}}(x)\cos\vartheta.
\end{aligned} \tag{8.105}$$

Therefore,

$$D_{H_{3,\vartheta}} = \{\psi \in D^*_{\check{H}}(0, \pi/2c),\ \psi \text{ satisfy } (8.105)\}.$$

Imposing the boundary conditions (8.105) on the functions (8.98) and using the asymptotics (8.104), we obtain the Green's function of the Hamiltonian $\hat{H}_{3,\vartheta}$,

$$\begin{aligned}
G(x, y; W) &= \Omega^{-1}(W)\, U_{3,\vartheta}(x; W) U_{3,\vartheta}(y; W)\\
&\quad + \frac{1}{c}\begin{cases} \tilde{U}_{3,\vartheta}(x; W) U_{3,\vartheta}(y; W),\ x > y,\\ U_{3,\vartheta}(x; W)\tilde{U}_{3,\vartheta}(y; W),\ x < y, \end{cases}
\end{aligned} \tag{8.106}$$

where

$$\begin{aligned}
\Omega(W) &= \frac{c\omega_{3,\vartheta}(W)}{\tilde{\omega}_{3,\vartheta}(W)},\ \omega_{3,\vartheta}(W) = f(W)\cos\vartheta - \sin\vartheta,\\
\tilde{\omega}_{3,\vartheta}(W) &= f(W)\sin\vartheta + \cos\vartheta,\ f(W) = \psi(\alpha)/2 + \psi(\beta)/2 + \mathbf{C},\\
U_{3,\vartheta}(x; W) &= u_1(x; W)\sin\vartheta + u_3(x; W)\cos\vartheta,\\
\tilde{U}_{3,\vartheta}(x; W) &= u_1(x; W)\cos\vartheta - u_3(x; W)\sin\vartheta,\\
V_1(x; W) &= -\frac{\omega(W)}{c}\left[\omega_{3,\vartheta}(W)\tilde{U}_{3,\vartheta}(x; W) + \tilde{\omega}_{3,\vartheta}(W) U_{3,\vartheta}(x; W)\right],
\end{aligned}$$

$U_{3,\vartheta}$ and $\tilde{U}_{3,\vartheta}$ are solutions of (8.93) real entire in W, $U_{3,\vartheta}$ satisfies the boundary condition (8.105), and the second summand on the right-hand side of (8.106) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty U_{3,\vartheta}(x; W)\xi(x)\mathrm{d}x,\ \xi \in D_r(0, \pi/2c) \cap D_{H_{3,\vartheta}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{3,\vartheta}$ ($\tilde{U} = \tilde{U}_{3,\vartheta}$), and therefore the spectra of $\hat{H}_{3,\vartheta}$ are simple.

The Green's function allows one to calculate the derivative of the spectral function, $\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega^{-1}(E + i0)$. The function $\Omega^{-1}(E)$ is real for any E where $\Omega(E) \neq 0$. That is why only the points $E_n(\vartheta)$ that satisfy the equation $\Omega(E_n(\vartheta)) = 0$ can provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_n Q^2_{\vartheta|n} \delta(E - E_n(\vartheta)),\ Q_{\vartheta|n} = \sqrt{-\Omega'(E_n(\vartheta))^{-1}}.$$

One can make some remarks on the spectrum structure. For the extension with $\vartheta = \pi/2$, we have $U_{3,\pi/2} = u_1$, and

$$\sigma'(E) = -(2\pi c)^{-1} \operatorname{Im}[\psi(\alpha) + \psi(\beta)]|_{W=E+i0}\,.$$

For $E = -c^2\tau^2 \le 0$, $\tau \ge 0$, $\lambda = i\tau$, the function $[\psi(\alpha) + \psi(\beta)]|_{W=E}$ is finite and real, so that we have $\sigma'(E) = 0$. For $E = c^2 p^2 > 0$, $p > 0$, $\lambda = p$, the function $\psi(\alpha)|_{W=E}$ is finite and real, so that we have (denoting the spectrum points by $\mathcal{E}_n$)

$$\sigma'(E) = \sum_{n\in\mathbb{Z}_+} 2\mathcal{E}_n^{1/2} \delta(E - \mathcal{E}_n),\ \mathcal{E}_n = c^2(1 + \nu + 2n)^2,\ n \in \mathbb{Z}_+\,.$$

The same results hold for the extension with $\vartheta = -\pi/2$. Note that the spectrum and complete set of eigenfunctions can be extracted from the case $g_1 \ge 3/4$ in the limit $\mu \to 0$.

Let us consider extensions with $|\vartheta| < \pi/2$. In this case,

$$\sigma'(E) = \sum_{n=n_{\min}} Q^2_{\vartheta|n} \delta(E - E_n(\vartheta)),\ Q_{\vartheta|n} = \sqrt{-\left[c f'_\vartheta(E_n(\vartheta))\right]^{-1}},$$

$$f_\vartheta(W) = f(W) - \tan\vartheta,\ f_\vartheta(E_n(\vartheta)) = \tan\vartheta,\ f'_\vartheta(E_n(\vartheta)) = f'(E_{\vartheta|n}) < 0.$$

The function $f(E)$ has the properties $f(E) \overset{E\to-\infty}{\longrightarrow} (1/2)\ln(|E|) + O(1)$, and

$$f(\mathcal{E}_n \pm 0) = \pm\infty,\ n \in \mathbb{Z}_+,\ \partial_\vartheta E_n(\vartheta) = \left[f'_\vartheta(E_n(\vartheta)) \cos^{2\vartheta}\right]^{-1} < 0.$$

Thus, for any $\vartheta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n \in \mathbb{Z}_+$, there exists one discrete level $E(\vartheta)$ monotonically increasing from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ as ϑ goes from $\pi/2 - 0$ to $-\pi/2 + 0$ (we set $E_{-1}(\pm\pi/2) = -\infty$). Furthermore, we find that $n_{\min} = 0$.

Thus, the simple spectra of $\hat{H}_{3,\vartheta}$ have the form spec $\hat{H}_{3,\vartheta} = \{E_n(\vartheta),\ n \in \mathbb{Z}_+\}$. The eigenfunctions $U_n(x) = Q_{\vartheta|n} U_{3,\vartheta}(x; E_{\vartheta|n})$ of each $\hat{H}_{3,\vartheta}$ form a complete orthonormalized system in $L^2(0, \pi/2c)$.

8.6.1.4 Subrange $g_2 \geq 3/4$, $g_1 < -1/4$, $\mu = i\varkappa$, $\varkappa > 0$

In this subrange, the functions $\psi_* \in D^*_{\check{H}}(0, \pi/2c)$ have the following asymptotics as $x \to 0$:

$$\psi_*(x) = a_1 u_{1\mathrm{as}}(x) + a_2 u_{2\mathrm{as}}(x) + O(x^{3/2}),$$
$$\psi_*'(x) = a_1 u_{1\mathrm{as}}'(x) + a_2 u_{2\mathrm{as}}'(x) + O(x^{1/2}),$$
$$u_{1\mathrm{as}}(x) = (cx)^{1/2+i\varkappa},\ u_{2\mathrm{as}}(x) = (cx)^{1/2-i\varkappa} = \overline{u_{1\mathrm{as}}(x)}.$$

Using these asymptotics and the fact that $[\chi_*, \psi_*](\pi/2c) = 0$, we obtain $\Delta_{H^+}(\psi_*) = 2i\varkappa c(\overline{a_1}a_1 - \overline{a_2}a_2)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1 = \mathrm{e}^{2i\theta}a_2$, $\theta \in \mathbb{S}(0, \pi)$. Thus, in the subrange under consideration, there exists a family of s.a. operators $\hat{H}_{4,\theta}$ parameterized by θ with domains $D_{H_{4,\theta}}$ that consist of functions from $D^*_{\check{H}}(0, \pi/2c)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{4,\theta\mathrm{as}}(x) + O(x^{3/2}),\ \psi'(x) = C\psi_{4,\theta\mathrm{as}}'(x) + O(x^{3/2}),$$
$$\psi_{4,\theta\mathrm{as}}(x) = \mathrm{e}^{i\theta}u_{1\mathrm{as}}(x) + \mathrm{e}^{-i\theta}u_{2\mathrm{as}}(x) = \overline{\psi_{4,\theta\mathrm{as}}(x)}. \tag{8.107}$$

Therefore,

$$D_{H_{4,\theta}} = \left\{\psi \in D^*_{\check{H}}(0, \pi/2c),\ \psi \text{ satisfy } (8.107)\right\}.$$

Imposing the boundary conditions (8.107) on the functions (8.98) and using the asymptotics (8.96) and (8.97), we obtain the Green's function of the Hamiltonian $\hat{H}_{4,\theta}$,

$$G(x, y; W) = \Omega^{-1}(W)U_{4,\theta}(x; W)U_{4,\theta}(y; W) + \frac{1}{4\varkappa c}\begin{cases} \tilde{U}_{4,\theta}(x; W)U_{4,\theta}(y; W),\ x > y, \\ U_{4,\theta}(x; W)\tilde{U}_{4,\theta}(y; W),\ x < y, \end{cases} \tag{8.108}$$

where

$$\Omega = 4i\varkappa c\frac{\omega_{4,\theta}(W)}{\tilde{\omega}_{4,\theta}(W)},\ \omega_{4,\theta}(W) = \mathrm{e}^{i\theta}a(W) + \mathrm{e}^{-i\theta}b(W),$$
$$\tilde{\omega}_{4,\theta}(W) = \mathrm{e}^{i\theta}a(W) - \mathrm{e}^{-i\theta}b(W),$$
$$U_{4,\theta}(x; W) = \mathrm{e}^{i\theta}u_1(x; W) + \mathrm{e}^{-i\theta}u_2(x; W).$$
$$\tilde{U}_{4,\theta}(x; W) = i[\mathrm{e}^{i\theta}u_1(x; W) - \mathrm{e}^{-i\theta}u_2(x; W)],$$
$$V_1(x; W) = \frac{\tilde{\omega}_{4,\theta}(W)}{2i\varkappa}U_{4\theta}(x; W) - \frac{\omega_{4,\theta}(W)}{2\varkappa}\tilde{U}_{4,\theta}(x; W).$$

We note that $U_{4,\theta}(x;W)$ and $\tilde{U}_{4,\theta}(x;W)$ are solutions of (8.93) real entire in W, $U_{4,\theta}(x;W)$ satisfies the boundary condition (8.107), and the second summand on the right-hand side of (8.108) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty U_{4,\theta}(x;W)\xi(x)\mathrm{d}x,\ \xi \in D_r(0,\pi/2c) \cap D_{4,\theta}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{4,\theta}$ ($\tilde{U} = \tilde{U}_{4,\theta}$), and therefore spectra of $\hat{H}_{4,\theta}$ are simple.

The derivative of the spectral function reads $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E+i0)$. For $W = E$, we have $b(E) = \overline{a(E)}$, so that $\Omega(E) = 4\varkappa c\cot\Theta(E)$, where

$$\Theta(E) = \theta + f(E),\ \ f(E) = \frac{1}{2i}[\ln(1+i\varkappa) - \ln(1-i\varkappa)] \\ + \frac{1}{2i}[\ln\Gamma(\alpha_2) + \ln\Gamma(\beta_2) - \ln\Gamma(\alpha_1) - \ln\Gamma(\beta_1)].$$

Only the points $E_n(\theta)$ obeying the equation $\cot\Theta(E_n(\theta)) = 0$, provide nonzero contributions to $\sigma'(E)$. Thus, we obtain

$$\sigma'(E) = \sum_{n\in\mathbb{Z}} Q^2_{\theta|n}\delta(E - E_n(\theta)),\ \Theta(E_n(\theta)) = \pi/2 + \pi n,\ n \in \mathbb{Z},$$

$$Q_{\theta|n} = \sqrt{(4\varkappa c\Theta'(E_n(\theta)))^{-1}},\ \Theta'(E_n(\theta)) = f'(E_n(\theta)) > 0.$$

The spectrum equation can be rewritten in the following form:

$$f(E_n(\theta)) = \pi/2 + \pi(n - \theta/\pi),\ n \in \mathbb{Z}.$$

Taking into account that

$$f(E) = \begin{cases} -(\varkappa/2)\ln(|E|/c^2) + O(1) \to -\infty,\ E \to -\infty, \\ \pi(E/4c^2)^{1/2} - (\varkappa/2)\ln(|E|/c^2) + O(1) \to \infty,\ E \to \infty, \end{cases}$$

we can see that for any $\theta \in [0,\pi)$, in each interval $(E_n(\pi) = E_{n-1}(0), E_n(0)]$, $n \in \mathbb{Z}$, there exists one discrete level $E_n(\theta)$ monotonically decreasing from $E_n(0)$ to $E_{n+1}(0) + 0$ as θ goes from 0 to $\pi - 0$. In particular, $E_n(0) > E_{n-1}(0)$.

Finally, we see that simple spectra of $\hat{H}_{4,\theta}$ read spec $\hat{H}_{4,\theta} = \{E_n(\theta),\ n \in \mathbb{Z}\}$. The eigenfunctions $U_n(x) = Q_{\theta|n}U_{4,\theta}(x;E_n(\theta))$, $n \in \mathbb{Z}$, of each $\hat{H}_{4,\theta}$ form a complete orthonormalized system in $L^2(0,\pi/2c)$.

We note that for $g_1 < -1/4$, the spectra of $\hat{H}_{4,\theta}$ are unbounded from below. For high negative energies, such spectra coincide with that of the Calogero problem with $\alpha = g_1$ and $k_0 \sim c$.

8.6.2 Range 2

In this range, we have

$$g_2 < 3/4.$$

In this range of g_2 and in the subrange $g_1 \geq 3/4$, all the results can be obtained from the above results by substitutions $x \to \pi/2c - x$ and $g_1 \longleftrightarrow g_2$.

In the subrange $g_1 < 3/4$ all the solutions are square-integrable and the deficiency indices of the initial symmetric operator $\hat{H}$ are $m_\pm = 2$. We omit further analysis of such a case because of the unwieldiness of the corresponding formulas.

We note that for any g_1 and g_2, the spectra of any s.a. extensions are not bounded from above and in the high positive energy limit asymptotically coincide with the energy spectrum of a free nonrelativistic particle of mass $m = 1/2$ in an infinite rectangular potential well of width $l = \pi/2c$.

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In this case,

$$V(x) = 4c^2[g_1 \tan^2(cx) + g_2 \tan(cx)], \quad x \in [-\pi/2c, \pi/2c], \tag{8.109}$$

and the corresponding Schrödinger equation is

$$\psi'' - 4c^2[g_1 \tan^2(cx) + g_2 \tan(cx)]\psi + W\psi = 0. \tag{8.110}$$

It is sufficient to consider only the case $c > 0$ and $g_2 \geq 0$ without loss of generality.

8.7.1 Self-adjoint Extension and Spectral Problem

Let us introduce a new variable $z = -e^{2icx}$ and new parameters μ, ν, and λ as follows:

$$\mu = \sqrt{g_1 - ig_2 + w}, \ \lambda = \sqrt{g_1 + ig_2 + w}, \ g_2 > 0,$$

$$\mu = \lambda = \sqrt{g_1 + w}, \ g_2 = 0, \ w = W/4c^2,$$

$$\nu = \begin{cases} \sqrt{4g_1 + 1/4}, \ g_1 \geq -1/16, \\ i\varkappa, \ \varkappa = \sqrt{4|g_1| - 1/4}, \ g_1 < -1/16, \end{cases} \qquad \nu^2 = 4g_1 + 1/4.$$

We note that the path $-\pi/2c \Longrightarrow \pi/2c$ of the variable x on the real axis corresponds to the path $1 \Longrightarrow 1$ of the variable z in the complex plane along (counter-clockwise) a circle $|z| = 1$ with the center at the origin.

In addition, we introduce new functions $\phi_{\xi_\mu}(z)$ instead of $\psi(x)$ in (8.110),

$$\psi(x) = (-z)^{\xi_\mu \mu}(1-z)^{1/2+\nu}\phi_{\xi_\mu}(z),\ \xi_\mu = \pm 1. \tag{8.111}$$

Then $\phi_{\xi_\mu}(z)$ satisfy the following equations:

$$\begin{aligned}
&z(1-z)d_z^2\phi_{\xi_\mu}(z) + [\gamma_{\xi_\mu} - (1 + \alpha_{\xi_\mu} + \beta_{\xi_\mu})z]d_z\phi_{\xi_\mu}(z) - \alpha_{\xi_\mu}\beta_{\xi_\mu}\phi_{\xi_\mu}(z) = 0,\\
&\alpha_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu + \lambda,\ \beta_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu - \lambda,\ \gamma_{\xi_\mu} = 1 + 2\xi_\mu\mu,
\end{aligned} \tag{8.112}$$

which have hypergeometric functions $F(\alpha, \beta; \gamma; z)$ as solutions; see [1, 20, 81], and also the appendix to this section.

Solutions of (8.110) can be obtained from solutions of (8.112) by the transformation (8.111). In what follows, we use several solutions of (8.110). Two of them, $u_1(x; W)$ and $u_2\,(x; W)$, have the form

$$\begin{aligned}
u_1\,(x; W) &= (-z)^{\mu}(1-z)^{1/2+\nu}\mathcal{F}(\alpha_1, \beta_1; \gamma_1; z)\\
&= -\frac{\mu}{\nu}A(-z)^{\mu}(1-z)^{1/2+\nu}\mathcal{F}(\alpha_1, \beta_1; \gamma_3; 1-z)\\
&\quad + \frac{\mu}{\nu}B(-z)^{\mu}(1-z)^{1/2-\nu}\mathcal{F}(\alpha_3, \beta_3; \gamma_4; 1-z) = u_1\,(x; W)|_{\nu\to-\nu}\,,\\
A &= \frac{\Gamma(2\mu)\Gamma(\gamma_4)}{\Gamma(\alpha_3)\Gamma(\beta_3)},\ B = \frac{\Gamma(2\mu)\Gamma(\gamma_3)}{\Gamma(\alpha_1)\Gamma(\beta_1)}\,;\\
u_2\,(x; W) &= (-z)^{-\mu}(1-z)^{1/2+\nu}\mathcal{F}(\alpha_2, \beta_2; \gamma_2; z)\\
&= C(-z)^{-\mu}(1-z)^{1/2+\nu}\mathcal{F}(\alpha_2, \beta_2; \gamma_3; 1-z)\\
&\quad + D(-z)^{-\mu}(1-z)^{1/2-\nu}\mathcal{F}(\alpha_4, \beta_4; \gamma_4; 1-z)\\
&= u_2\,(x; W)|_{\nu\to-\nu} = u_1\,(x; W)|_{\mu\to-\mu}\,,\\
C &= \frac{\Gamma(\gamma_2)\Gamma(-2\nu)}{\Gamma(\alpha_4)\Gamma(\beta_4)},\ D = \frac{\Gamma(\gamma_2)\Gamma(2\nu)}{\Gamma(\alpha_2)\Gamma(\beta_2)},\ AD + BC = 1,
\end{aligned} \tag{8.113}$$

where

$$\begin{aligned}
&\alpha_{1,2} = 1/2 \pm \mu + \nu + \lambda,\ \beta_{1,2} = 1/2 \pm \mu + \nu - \lambda,\\
&\alpha_{3,4} = 1/2 \pm \mu - \nu + \lambda,\ \beta_{3,4} = 1/2 \pm \mu - \nu - \lambda,\\
&\gamma_{1,2} = 1 \pm 2\mu,\ \gamma_{3,4} = 1 \pm 2\nu,
\end{aligned}$$

and the function $\mathcal{F}(\alpha, \beta; \gamma; z)$ is the analytic continuation of the hypergeometric series in the complex plane with a cut along the real semiaxis $x \geq 1$ and is given, for example, by the Barnes integral; see, e.g., [164] and the appendix to this section.

Note that all the points z: $|z| = 1$, $z \neq 1$, belong to analyticity domains of the functions $(-z)^\alpha$, $(1-z)^\alpha$, and $\mathcal{F}(\alpha, \beta; \gamma; z)$, so that $u_1(x; W)$ and $u_2(x; W)$ are indeed solutions of (8.110) for $x \in (-\pi/2c, \pi/2c)$.

The asymptotic behavior of special functions in solutions (8.113) are well known; see, e.g., [1, 20, 81]. We use these asymptotics and we restrict ourselves by the range $0 < \operatorname{Im} w < b_0$,

$$b_0 = \min\left(t\sqrt{g_2},\ g_2,\ 2t\sqrt{g_2}\varkappa\right),\ t = \sqrt{\sqrt{2}/8 - 1/8},$$

which is enough for our purposes. Considering the strip $0 < \operatorname{Im} w < b_0$, where $\alpha_k, \beta_k, \gamma_i \notin \mathbb{Z}_-$, $k = 1, 2, 3, 4$, $i = 1, 2, 3$, we obtain the following: For $x = -\pi/2c + \delta$, $\delta \to 0$, we have

$$u_1 = \left[-\frac{\mu}{\nu} A \mathrm{e}^{-i\pi(1/4+\mu+\nu/2)}(2c\delta)^{1/2+\nu} + \frac{\mu}{\nu} B \mathrm{e}^{-i\pi(1/4+\mu-\nu/2)}(2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta),$$
$$u_2 = \left[\mathrm{e}^{-i\pi(1/4-\mu+\nu/2)} C (2c\delta)^{1/2+\nu} + \mathrm{e}^{-i\pi(1/4-\mu-\nu/2)} D (2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta).$$

For $x = \pi/2c - \delta$, $\delta \to 0$, we have

$$u_1 = \left[-\frac{\mu}{\nu} A \mathrm{e}^{i\pi(1/4+\mu+\nu/2)}(2c\delta)^{1/2+\nu} + \frac{\mu}{\nu} B \mathrm{e}^{i\pi(1/4+\mu-\nu/2)}(2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta),$$
$$u_2 = \left[C \mathrm{e}^{i\pi(1/4-\mu+\nu/2)}(2c\delta)^{1/2+\nu} + D \mathrm{e}^{i\pi(1/4-\mu-\nu/2)}(2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta).$$

Regarding $\operatorname{Wr}(u_1, u_2) = -4i\mu c$, solutions u_1 and u_2 form a fundamental set of solutions of (8.110).

Another set of solutions of (8.110) with definite asymptotics at one of the endpoints are solutions $V_1(x; W)$,

$$V_1 = -\frac{\nu}{\mu} D \mathrm{e}^{i\pi(1/4+\mu+\nu/2)} u_1(x; W) + B \mathrm{e}^{i\pi(1/4-\mu+\nu/2)} u_2(x; W),$$
$$V_1 \overset{\delta \to 0}{=} \begin{cases} \left[F_1 (2c\delta)^{1/2+\nu} + P_1 (2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta),\ x = \pi/2c - \delta \\ (2c\delta)^{1/2+\nu}\tilde{O}(\delta),\ x = -\pi/2c + \delta \end{cases},$$
$$F_1 = i\mathrm{e}^{i\pi\nu}\left(AD\mathrm{e}^{2i\pi\mu} + BC\mathrm{e}^{-2i\pi\mu}\right) = -\frac{\mathrm{e}^{-i\pi\nu}\cos(2\pi\mu) + \mathrm{e}^{i\pi\nu}\cos(2\pi\lambda)}{\sin(2\pi\nu)},$$
$$P_1 = -iBD\left(\mathrm{e}^{2i\pi\mu} - \mathrm{e}^{-2i\pi\mu}\right) = \frac{2\pi\Gamma(2\nu)\Gamma(\gamma_3)}{\Gamma(\alpha_1)\Gamma(\beta_1)\Gamma(\alpha_2)\Gamma(\beta_2)};$$

solutions $V_2(x; W)$

$$V_2 = -\frac{\nu}{\mu} D e^{-i\pi(1/4+\mu+\nu/2)} u_1(x;W) + B e^{-i\pi(1/4-\mu+\nu/2)} u_2(x;W),$$

$$V_2 \overset{\delta\to 0}{=} \begin{cases} (2c\delta)^{1/2+\nu}\tilde{O}(\delta), \ x = \pi/2c - \delta \\ \left[-F_2(2c\delta)^{1/2+\nu} + P_1(2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta), \ x = -\pi/2c + \delta \end{cases},$$

$$F_2 = i e^{-i\pi\nu}\left(AD e^{-2i\pi\mu} + BC e^{2i\pi\mu}\right) = \frac{e^{i\pi\nu}\cos(2\pi\mu) + e^{-i\pi\nu}\cos(2\pi\lambda)}{\sin(2\pi\nu)};$$

solutions $V_3(x;W)$

$$V_3 = \frac{\nu}{\mu} C e^{i\pi(1/4+\mu-\nu/2)} u_1(x;W) + A e^{i\pi(1/4-\mu-\nu/2)} u_2(x;W),$$

$$V_3 \overset{\delta\to 0}{=} \begin{cases} \left[F_3(2c\delta)^{1/2+\nu} + F_2(2c\delta)^{1/2-\nu}\right]\tilde{O}(\delta), \ x = \pi/2c - \delta \\ (2c\delta)^{1/2-\nu}\tilde{O}(\delta), \ x = -\pi/2c + \delta \end{cases},$$

$$F_3 = -iAC\left(e^{2i\pi\mu} - e^{-2i\pi\mu}\right) = \frac{2\pi\Gamma(-2\nu)\Gamma(\gamma_4)}{\Gamma(\alpha_3)\Gamma(\beta_3)\Gamma(\alpha_4)\Gamma(\beta_4)}.$$

For these solutions, we have

$$\begin{aligned} &\mathrm{Wr}(V_1, V_3) = -4c\nu, \ \mathrm{Wr}(V_1, V_2) = -4c\nu P_1 = -\omega(W), \\ &\mathrm{Wr}(V_3, V_2) = -4c\nu F_2 = -\omega_2(W), \\ &V_2(x;W) = \frac{1}{4c\nu}\left[\omega(W)V_3(x;W) - \omega_2(W)V_1(x;W)\right]. \end{aligned}$$

For $g_1 \geq -1/16$ ($\nu \geq 0$), all solutions V_i are real entire in W, and for $g_1 < -1/16$ ($\nu = -i\varkappa$), they are entire in W and $\overline{V_3(x;E)} = V_1(x;E)$.

The initial symmetric operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}(-\pi/2c, \pi/2c)$ and its adjoint $\hat{H}^+$ on the domain $D_{H^+} = D^*_{\check{H}}(-\pi/2c, \pi/2c)$. The solutions V_1 and V_2 form a fundamental set of solutions of (8.110) for $\operatorname{Im} w > 0$. Taking their asymptotics into account, one can see the following:

For $g_1 \geq 3/16$ ($\nu \geq 1$), (8.110) has no square-integrable solutions on $[-\pi/2c, \pi/2c]$, so that in this region, the deficiency indices of $\hat{H}$ are zero, which implies that the operator $\hat{H}^+$ is s.a. and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

For $g_1 < 3/16$ ($\operatorname{Re}\nu < 1$), any solution of (8.110) is square-integrable on $[-\pi/2c, \pi/2c]$, so that in this region, the deficiency indices are equal, $m_\pm = 2$, which implies that there exists a $U(2)$ family of s.a. extensions $\hat{H}_U$ of $\hat{H}$. Their study in detail is an enormous problem. Below, we consider only the case $g_1 \geq 3/16$ in detail.

Asymptotics of functions $\psi_* \in D^*_{\check{H}}(-\pi/2c, \pi/2c)$ as $x \to -\pi/2c$ can be found with the help of the method used in Sect. 8.6. First, we note that any $\psi_* \in D^*_{\check{H}}(-\pi/2c, \pi/2c)$ belongs also to $D^*_{\check{H}}(-\pi/2c, 0)$; in particular,

$$\psi_* \in D^*_{\check{H}}(-\pi/2c, \pi/2c) \Longrightarrow \psi_*, \check{H}\psi_* \in L^2(-\pi/2c, 0).$$

Due to the fact that the potential (8.109) can be represented as $V(x) = 4g_1\delta^{-2} - 4cg_2\delta^{-1} + v(x)$, $x = -\pi/(2c) + \delta$, where $v(x)$ is a bounded function on the segment $[-\pi/2c, 0]$, functions $\psi_*(x)$ can be considered on the interval $(-\pi/2c, 0]$ as solutions of the equation

$$-\psi_*''(x) + (4g_1\delta^{-2} - 4cg_2\delta^{-1})\psi_*(x) = \eta(x),$$
$$\eta(x) = \check{H}\psi_*(x) - v(x)\psi_*(x) \in L^2(-\pi/2c, 0).$$

The asymptotic behavior of such solutions as $\delta \to 0$ was studied in Sect. 7.3.3. For $g_1 \geq 3/16$, we have

$$\psi_*(x) = O(\delta^{3/2}),\ \psi_*'(x) = O(\delta^{1/2}),\ \delta \to 0\ (x \to -\pi/2c),$$

with logarithmic accuracy for $g_1 = 3/16$.

In the same manner, we obtain for $x \to \pi/2c$

$$\psi_*(x) = O(\delta^{3/2}),\ \psi_*'(x) = O(\delta^{1/2}),\ \delta = \pi/(2c) - x \to 0,$$

with logarithmic accuracy for $g_1 = 3/16$.

The Green's function of the s.a. operator $\hat{H}_1$ has the form

$$G(x, y; W) = \omega^{-1}(W) \begin{cases} V_2(x; W)V_1(y; W),\ x > y, \\ V_1(x; W)V_2(y; W),\ x < y. \end{cases}$$

Let us consider the guiding functional

$$\Phi(\xi; W) = \int_{-\pi/2c}^{\pi/2c} \mathrm{d}x\, V_1(x; W)\xi(x),\ \xi \in \mathcal{D}_r(-\pi/2c, \pi/2c) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = V_1$ ($\tilde{U} = V_2$), and therefore the spectrum of $\hat{H}_1$ is simple.

The derivative of the spectral function has the form

$$\sigma'(E) = \frac{V_2(x_0; E)}{V_1(x_0; E)} \operatorname{Im}[\pi\omega(E + i0)]^{-1}. \tag{8.114}$$

For $\nu \neq n/2$, the function $V_2(x_0; W)$ can be represented as $V_2(x_0; W) = -F_2V_1(x_0; W) + (\omega/4c\nu)V_3(x_0; W)$, so that expression (8.114) is simplified:

$$\sigma'(E) = -F_2|_{W=E} \operatorname{Im}[\pi\omega(E + i0)]^{-1}.$$

It is easy to see that $\sigma'(E)$ is continuous in ν, so that it is enough to calculate $\sigma'(E)$ for $\nu \neq n/2$ only.

Because $\omega(E)$ is real, $\sigma'(E)$ can be nonzero only at the zero points of $\omega(E)$, i.e., at the points $\beta_2 = -n, n \in \mathbb{Z}_+$ ($\Gamma(\beta_2) = \infty$), so that we obtain in the standard way,

$$\sigma'(E) = \sum_{n \in \mathbb{Z}_+} Q_n^2 \delta(E_n), \; Q_n = \frac{|\Gamma(\alpha_2)||\mu_n| \mathrm{e}^{-\pi \operatorname{Im} \mu_n}}{\Gamma(\gamma_3)} \sqrt{\frac{\Gamma(\gamma_3 + n)}{4\pi c n! \operatorname{Re} \mu_n}},$$
$$E_n = c^2 \left[(1/2 + n + \nu)^2 - 4g_1 - 4g_2^2 (1/2 + n + \nu)^{-2} \right],$$
$$\mu_n = \sqrt{g_1 - i g_2 + E_n / 4c^2}.$$

Thus, the simple spectrum of $\hat{H}_1$ is given by spec $\hat{H}_1 = \{E_n, \; n \in \mathbb{Z}_+\}$. The set of eigenfunctions $U_n(x) = Q_n V_1(x; E_n)$, $n \in \mathbb{Z}_+$, forms a complete orthonormalized system in $L^2(-\pi/2c, \pi/2c)$.

Note that the spectrum of $\hat{H}_1$ coincides asymptotically (as $n \to \infty$) with the spectrum of the Hamiltonian of free non-relativistic particle with mass $m = 1/2$ in an infinite rectangular potential well of width $l = \pi/c$.

8.7.2 *Appendix*

The function $\mathcal{F}(\alpha, \beta; \gamma; z)$ is the analytic continuation of the hypergeometric series in the complex plane with a cut along real semiaxis $x \geq 1$ and is given by the Barnes integral; see [164]. We used three relations for the function $\mathcal{F}(\alpha, \beta; \gamma; z)$:

$$\mathcal{F}(\alpha, \beta; \gamma; z) = (1 - z)^{\gamma - \alpha - \beta} \mathcal{F}(\gamma - \alpha, \gamma - \beta; \gamma; z), \tag{8.115}$$

$$\lim_{\gamma \to -n} \Gamma^{-1}(\gamma) \mathcal{F}(\alpha, \beta; \gamma; z) = \frac{\Gamma(\alpha + n + 1)\Gamma(\beta + n + 1)}{\Gamma(\alpha)\Gamma(\beta)(n+1)!} \times z^{n+1} \mathcal{F}(\alpha + n + 1, \beta + n + 1; n + 2; z), \tag{8.116}$$

$$\begin{aligned} &\mathcal{F}(\alpha, \beta; \gamma; z) \\ &\quad = \frac{\Gamma(\gamma)\Gamma(\beta - \alpha)}{\Gamma(\beta)\Gamma(\gamma - \alpha)} (-z)^{-\alpha} \mathcal{F}(1 + \alpha - \gamma, \alpha; 1 + \alpha - \beta; z^{-1}) + (\alpha \leftrightarrow \beta), \\ &\mathcal{F}(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)\Gamma(\gamma - \beta)} \mathcal{F}(\alpha, \beta; 1 + \alpha + \beta - \gamma; 1 - z) \\ &\quad + \frac{\Gamma(\gamma)\Gamma(\alpha + \beta - \gamma)}{\Gamma(\alpha)\Gamma(\beta)} (1 - z)^{\gamma - \alpha - \beta} \mathcal{F}(\gamma - \alpha, \gamma - \beta; 1 + \gamma - \alpha - \beta; 1 - z). \end{aligned} \tag{8.117}$$

For any complex u, the function u^α is defined as the principal value of the power function,

$$u^\alpha = |u|^\alpha \mathrm{e}^{i\phi_u \alpha} = \mathrm{e}^{\alpha \ln |u|} \mathrm{e}^{i\phi_u \alpha}, \; u = |u| \mathrm{e}^{i\phi_u}, \; |\phi_u| < \pi.$$

The function u^α is analytic in the complex plane u with the cut along negative real semiaxis and obeys the following relations:

$$(1/u)^\alpha = u^{-\alpha},\ u^\alpha u^\beta = u^{\alpha+\beta},\ \overline{u^\alpha} = (\overline{u})^{\overline{\alpha}},$$
$$(-u)^\alpha (1-1/u)^\beta = (-u)^{\alpha-\beta}(1-u)^\beta.$$

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In this case,

$$V(x) = 4c^2 g_1 \tan h^2(cx) + 4c^2 g_2 \tan h(cx),\quad x \in \mathbb{R}, \tag{8.118}$$

and the corresponding Schrödinger equation is

$$\psi'' - \left[4c^2 g_1 \tan h^2(cx) + 4c^2 g_2 \tan h(cx)\right]\psi + W\psi = 0. \tag{8.119}$$

It is sufficient to consider only the case $g_2 \geq 0$, $c > 0$ without loss of generality.

The potential (8.118) is known as the *Rosen–Morse potential*; see [134].

Let us introduce a new variable z and new functions $\varphi_\pm$, instead of x and $\psi(x)$ in (8.119),

$$z = \frac{1}{2}\left[1 - \tan h(cx)\right],\ z \in [0,1],\ \psi = z^{\pm\mu}(1-z)^\nu \phi_\pm(z),$$
$$\mu = \sqrt{g_1 + g_2 - w},\ \nu = \sqrt{g_1 - g_2 - w},\ \lambda = \sqrt{4g_1 + 1/4},\ w = W/4c^2.$$

If $\operatorname{Im} w \geq 0$, then

$$g_1 + g_2 - w = \rho_1 e^{-i\theta_1},\ g_1 - g_2 - w = \rho_2 e^{-i\theta_2},$$
$$0 \leq \theta_1, \theta_2 \leq \pi,$$
$$\mu = \sqrt{\rho_1} e^{-i\theta_1/2},\ \nu = \sqrt{\rho_2} e^{-i\theta_2/2},\ \operatorname{Re}\mu > 0,\ \operatorname{Re}\nu > 0,$$
$$\lambda = \begin{cases} \sqrt{4g_1 + 1/4},\ g_1 \geq -1/16, \\ i\sigma,\ \sigma = \sqrt{4|g_1| - 1/4} > 0,\ g_1 < -1/16, \end{cases}$$

and $\phi_\pm(z)$ satisfy the equation

$$z(1-z)d_z^2\phi_\pm(z) + [1 \pm 2\mu - (2 \pm 2\mu + 2\nu)z]d_z\phi_\pm(z)$$
$$- (1/2 \pm \mu + \nu + \lambda)(1/2 \pm \mu + \nu - \lambda)\varphi_\pm(z) = 0, \tag{8.120}$$

which has hypergeometric functions $F(\alpha, \beta; \gamma; z)$ as solutions, see [1, 20, 81].

Solutions $\psi(x)$ of (8.119) can be obtained from solutions of (8.120) by the above transformations. We use solutions $u_1(x;W)$ and $u_2(x;W)$ in what follows,

$$u_1(x;W) = z^{\mu}(1-z)^{\nu}F(\alpha,\beta;\gamma;z) = u_1(x;W)|_{\nu\to-\nu},$$
$$u_2(x;W) = z^{-\mu}(1-z)^{\nu}F(\alpha_1,\beta_1;\gamma_1;z) = u_2(x;W)|_{\nu\to-\nu},$$
$$\alpha = 1/2+\mu+\nu+\lambda,\ \beta = 1/2+\mu+\nu-\lambda,\ \gamma = 1+2\mu,$$
$$\alpha_1 = \alpha|_{\mu\to-\mu} = 1/2-\mu+\nu+\lambda,\ \beta_1 = \beta|_{\mu\to-\mu} = 1/2-\mu+\nu-\lambda,$$
$$\gamma_1 = \gamma|_{\mu\to-\mu} = 1-2\mu,\ u_2(x;W) = u_1(x;W)|_{\mu\to-\mu}.$$

Another set of solutions can be obtained as follows. We introduce a new variable z_1 and new functions $\tilde{\phi}_{\pm}$,

$$z_1 = \frac{1}{2}[1+\tan h(cx)] = 1-z,\ z_1\in[0,1],$$
$$\psi(x) = z_1^{\mu}(1-z_1)^{\pm\nu}\tilde{\phi}_{\pm}(z_1).$$

The new functions satisfy the same type of equation (8.120),

$$z_1(1-z_1)d_{z_1}^2\tilde{\phi}_{\pm}(z_1) + [1\pm 2\nu-(2+2\mu\pm 2\nu)z]d_{z_1}\tilde{\phi}_{\pm}(z_1)$$
$$-(1/2+\mu\pm\nu+\lambda)(1/2+\mu\pm\nu-\lambda)\tilde{\phi}_{\pm}(z_1) = 0.$$

In such way, we obtain two additional solutions of (8.119),

$$v_1(x;W) = z^{\mu}(1-z)^{\nu}F(\alpha,\beta;\gamma_2;1-z),\ \gamma_2 = 1+2\nu,$$
$$v_2(x;W) = z^{\mu}(1-z)^{-\nu}F(\alpha_2,\beta_2;\gamma_3;1-z),\ \gamma_3 = 1-2\nu,$$
$$\alpha_2 = 1/2+\mu-\nu+\lambda,\ \beta_2 = 1/2+\mu-\nu-\lambda,$$
$$\alpha_3 = \alpha_2|_{\mu\to-\mu} = 1/2-\mu-\nu+\lambda,\ \beta_3 = \beta_2|_{\mu\to-\mu} = \frac{1}{2}-\mu-\nu-\lambda,$$
$$v_{1,2}(x;W) = v_{1,2}(x;W)|_{\mu\to-\mu},\ v_2(x;W) = v_1(x;W)|_{\nu\to-\nu}.$$

There exist relations between the four solutions introduced (see [1, 20, 81]),

$$u_1 = \frac{\Gamma(\gamma)\Gamma(-2\nu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}v_1 + \frac{\Gamma(\gamma)\Gamma(2\nu)}{\Gamma(\alpha)\Gamma(\beta)}v_2,$$
$$v_1 = \frac{\Gamma(\gamma_2)\Gamma(-2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_1 + \frac{\Gamma(\gamma_2)\Gamma(2\mu)}{\Gamma(\alpha)\Gamma(\beta)}u_2.$$

These relations are useful for obtaining asymptotics of the functions u_1 and v_1: As $x\to\infty$, $z = \mathrm{e}^{-2cx}\tilde{O}(\mathrm{e}^{-2cx})\to 0$, $\operatorname{Im} W > 0$, we have

$$u_1(x;W) = \mathrm{e}^{-2c\mu x}\tilde{O}(\mathrm{e}^{-2cx})\to 0,$$
$$v_1(x;W) = \frac{\Gamma(\gamma_2)\Gamma(2\mu)}{\Gamma(\alpha)\Gamma(\beta)}\mathrm{e}^{2c\mu x}\tilde{O}(\mathrm{e}^{-2cx})\to\infty.$$

As $x \to -\infty$, $1 - z = \mathrm{e}^{-2c|x|}\tilde{O}(\mathrm{e}^{-2c|x|}) \to 0$, $\operatorname{Im} W > 0$, we have

$$u_1(x;W) = \frac{\Gamma(\gamma)\Gamma(2\nu)}{\Gamma(\alpha)\Gamma(\beta)}\mathrm{e}^{2c\mu|x|}\tilde{O}(\mathrm{e}^{-2c|x|}) \to \infty,$$

$$v_1(x;W) = \mathrm{e}^{-2c\mu|x|}\tilde{O}(\mathrm{e}^{-2c|x|}) \to 0.$$

For $\operatorname{Im} W > 0$, solutions u_1 and v form a fundamental set of solutions because

$$\operatorname{Wr}(u_1, v_1) = \frac{2c\Gamma(\gamma)\Gamma(\gamma_2)}{\Gamma(\alpha)\Gamma(\beta)} = \omega(W).$$

As usual, starting with the s.a. differential operation $\check{H}$, we construct the initial symmetric operator $\hat{H}$ defined on the domain $\mathcal{D}(\mathbb{R})$. Its adjoint $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R})$.

Because the potential $V(x)$ is bounded on $\mathbb{R}$, $|V(x)| \leq 4c^2(|g_1| + |g_2|)$, the asymmetry form $\Delta_{H^+}(\psi_*)$ vanishes on functions ψ_* from $D^*_{\check{H}}(\mathbb{R})$,

$$\Delta_{H^+}(\psi_*) = [\psi_*, \psi_*]|_{-\infty}^{\infty} = 0, \quad \forall \psi_* \in D^*_{\check{H}}(\mathbb{R}),$$

according to Theorem 7.1. This implies that the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$. On the other hand, any linear combination of the fundamental set u_1 and v is not square-integrable at $\operatorname{Im} W \neq 0$. The latter means that the deficiency indices of $\hat{H}$ are zero, which matches the previous conclusion.

It is convenient to introduce two additional independent and real entire solutions of (8.119), $T_k(x;W)$, $k = 1, 2$, for which

$$T_k^{(l-1)}(0;W) = \delta_{kl},\ k, l = 1, 2,\ \operatorname{Wr}(T_1.T_2) = 1.$$

One can see that

$$u_1(x;W) = u_1(0;W)T_1(x;W) + u_1'(0;W)T_2(x;W),$$

$$v_1(x;W) = v_1(0;W)T_1(x;W) + v_1'(0;W)T_2(x;W),$$

$$T_1(x;W) = \omega^{-1}(W)[v_1'(0;W)u_1(x;W) - u_1'(0;W)v_1(x;W)],$$

$$T_2(x;W) = \omega^{-1}(W)[-v_1(0;W)u_1(x;W) + u_1(0;W)v_1(x;W)].$$

The Green's function of the operator $\hat{H}_1$ has the form

$$G(x, y; W) = \omega^{-1}(W)\begin{cases} u_1(x;W)v_1(y;W), & x > y, \\ v_1(x;W)u_1(y;W), & x < y. \end{cases}$$

This allows us to find the matrix $M_{kl}(0;W)$,

$$M_{kl}(0;W) = \omega^{-1}(W)K_{kl}(W) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$$K_{kl}(W) = \begin{pmatrix} v_1(0;W)u_1(0;W) & v_1(0;W)u_1'(0;W) \\ v_1(0;W)u_1'(0;W) & v_1'(0;W)u_1'(0;W) \end{pmatrix},$$

see Sect. 5.3.2, and the derivative of the matrix spectral function

$$\sigma'_{kl}(E) = \pi^{-1} \operatorname{Im}\left[\omega^{-1}(E + i0) K_{kl}(E + i0)\right]. \tag{8.121}$$

As the set of guiding functionals, we chose

$$\Phi_k(\xi; W) = \int_{\mathbb{R}} \mathrm{d}x\, T_k(x; W)\, \xi(x), \; \xi \in D^*_{\check{H}}(\mathbb{R}) \cap D(\mathbb{R}).$$

Let $E < 4c^2(g_1 - g_2)$. In this case the functions $K_{kl}(E)$ are finite and real and the function $\omega(E)$ is real. That is why only the points E obeying the equation $\omega(E) = 0$ can provide nonzero contributions to the right-hand side of (8.121). One can easily see that the latter equation has solutions only for $g_1 > -1/16$. In that case, parameters α, γ, and γ_2 are real and positive and β is real, so that

$$\begin{aligned}
&\omega(E) = 0 \Longrightarrow \beta = \beta_n = -n, \; n \in \mathbb{Z}_+ \Longrightarrow \\
&\sqrt{a_n} + \sqrt{a_n + 2g_2} = \lambda - (n + 1/2), \\
&a_n = g_1 - g_2 - E_n/(4c^2) > 0.
\end{aligned} \tag{8.122}$$

It follows from (8.122) that

$$\begin{aligned}
&\lambda - (n + 1/2) - \sqrt{a_n + 2g_2} > 0, \\
&\sqrt{a_n} = \frac{1}{2}[\lambda - (n + 1/2)] - \frac{g_2}{\lambda - (n + 1/2)} \geq 0.
\end{aligned} \tag{8.123}$$

Finally, we obtain

$$E_n = 4c^2 g_1 - \left(\frac{2cg_2}{\lambda - (n + 1/2)}\right)^2 - c^2[\lambda - (n + 1/2)]^2.$$

One can verify that $g_1 - g_2 - E_n/4c^2 > 0$, so that all the discrete levels are situated below the continuous spectrum, which consists of the continuous levels $E \geq 4c^2(g_1 - g_2)$; see below.

Substituting E_n in the second inequality (8.123), we obtain $n < \lambda - \sqrt{2g_2} - 1/2$. This inequality implies that there exist $n_{\max} + 1$ discrete levels, where

$$n_{\max} = \begin{cases} [g], & g > [g], \\ [g] - 1, & g = [g], \end{cases} \qquad g = \lambda - \sqrt{2g_2} - 1/2.$$

The condition $g_1 > g_2/2 + \sqrt{g_2/8}$ provides the existence at least of one energy level.

Using the relations

$$v_1(x;W) = \frac{\Gamma(\gamma_2)\Gamma(-2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)} u_1(x;W)\Big|_{\beta=-n},$$
$$\operatorname{Im}\Gamma(\beta) = (-1)^n \pi b_n \delta(E-E_n) \text{ for } E_{n+1} < E < E_{n-1},$$
$$b_n = \frac{\lambda-(n+1/2)}{2n!\sqrt{a_n(a_n+2g_2)}},$$

we obtain

$$\sigma'_{kl}(E) = \begin{cases} 0, \ g_1 \le g_2/2 + \sqrt{g_2/8}, \\ \sum_{n=0}^{k} Q_n^2 \delta(E-E_n) e_{n,k} \otimes e_{n,l}, \ g_1 > g_2/2 + \sqrt{g_2/8}, \end{cases}$$
$$Q_n^2 = b_n c_n, \ c_n = \frac{\Gamma(\alpha)}{2c\Gamma(\alpha_1)} \left| \frac{\Gamma(-2\mu)}{\Gamma(-n-2\mu)} \right| \Big|_{E\to E_n},$$
$$e_{n,1} = u_1(0;E_n), \ e_{n,2} = u_1'(0;E_n). \tag{8.124}$$

It follows from (8.124) that in the range $E < 4c^2(g_1 - g_2)$, there can be only discrete levels (if they exist).

Let $4c^2(g_1-g_2) \le E < 4c^2(g_1+g_2)$. In this case μ and γ are real and positive, and

$$\nu = -i|\nu|, \ |\nu| = \sqrt{g_2 - g_1 + E/4c^2}, \ \overline{\nu} = -\nu,$$
$$\alpha, \beta \ne -n, \ n \in \mathbb{Z}_+, \ 0 < |\Gamma(\gamma_2)| < \infty,$$
$$\overline{\alpha} = \begin{cases} \alpha_2, \ g_1 \ge -1/16, \\ \beta_2, \ g_1 < -1/16, \end{cases} \quad \overline{\beta} = \begin{cases} \beta_2, \ g_1 \ge -1/16, \\ \alpha_2, \ g_1 < -1/16. \end{cases}$$

In turn, this implies that $u_1 = \overline{u_1}$ and $\omega(E) \ne 0, \infty$.

Let us introduce the notation

$$\omega^{-1}(E) v_1(x;E) = \tilde{v}_1(x;E), \ \operatorname{Im}\tilde{v}_1(x;E) = I(x;E).$$

It follows that $\mathrm{Wr}(u_1, \tilde{v}_1) = 1 \Longrightarrow \operatorname{Im}\mathrm{Wr}(u_1, \tilde{v}_1) = 0$, so that

$$\frac{I(x;E)}{u_1(x;E)} = \frac{I'(x;E)}{u_1'(x;E)}. \tag{8.125}$$

Since u_1 and u_1' cannot vanish simultaneously, both sides of the relation (8.125) are finite for any x and E.

Then we obtain

$$\sigma'_{kl}(E) = \rho(E) e_k(E) \otimes e_l(E), \ \rho(E) = \frac{I(0;E)}{\pi u_1(0;E)},$$
$$e_1(E) = u_1(0;E), \ e_2(E) = u_1'(0;E),$$

where $\rho(E)$ is a smooth function of E, so that the spectrum of $\hat{H}_1$ is continuous.

Let $E \geq 4c^2(g_1 + g_2)$. For these energies we have

$$\mu = -i|\mu|,\ |\mu| = \sqrt{E - g_1 - g_2},\ \nu = -i|\nu|,\ |\nu| = \sqrt{|\mu|^2 + 2g_2},$$
$$\alpha, \beta, \gamma, \gamma_2 \neq n,\ n \in \mathbb{Z}_+,\ \omega(E) \neq 0, \infty,$$

and $u_1(x; E)$ and $v_1(x; E)$ form a fundamental set of solutions.

Then

$$\sigma'_{kl}(E) = \operatorname{Im}\left[\frac{K_{kl}(E)}{\pi\omega(E)}\right] = \rho_{kl}(E),$$

where $\rho_{kl}(E)$ are smooth functions of E, so that the spectrum of $\hat{H}_1$ is continuous.

Finally, we obtain

$$\operatorname{spec} \hat{H}_1 = \begin{cases} [4c^2(g_1 - g_2), \infty),\ g_1 \leq g_2/2 + \sqrt{g_2/8}, \\ [4c^2(g_1 - g_2), \infty) \cup \{E_n, n = 0, 1, \ldots, n_{\max}\},\ g_1 > g_2/2 + \sqrt{g_2/8}. \end{cases}$$

We note that $E_n < 4c^2(g_1 - g_2)$; all the discrete levels are situated below the continuous spectrum (and certainly above the minimum of the potential energy $-c^2 g_2^2/g_1$).

Inversion formulas for different ranges of parameters g_1 and g_2 are listed below. Namely, for any $\psi(x) \in L^2(\mathbb{R})$, we have

(1) $g_1 \leq g_2/2 + \sqrt{g_2/8}$,

$$\psi(x) = \int_{4c^2(g_1-g_2)}^{4c^2(g_1+g_2)} \Phi(E) u_1(x; E) \rho(E) \mathrm{d}E$$
$$+ \int_{4c^2(g_1+g_2)}^{\infty} \Phi_i(E) \rho_{ij}(E) T_j(x; E) \mathrm{d}E,$$

$$\Phi(E) = \int_{\mathbb{R}} u_1(x; E) \psi(x) \mathrm{d}x,\ 4c^2(g_1 - g_2) \leq E < 4c^2(g_1 + g_2),$$

$$\Phi_i(E) = \int_{\mathbb{R}} T_i(x; E) \psi(x) \mathrm{d}x,\ E \geq 4c^2(g_1 + g_2),$$

$$\int_{\mathbb{R}} |\psi(x)|^2 \mathrm{d}x = \int_{4c^2(g_1-g_2)}^{4c^2(g_1+g_2)} |\Phi(E)|^2 \rho(E) \mathrm{d}E$$
$$+ \int_{4c^2(g_1+g_2)}^{\infty} \overline{\Phi_i(E)} \rho_{ij}(E) \Phi_j(E) \mathrm{d}E.$$

(2) $g_1 > g_2/2 + \sqrt{g_2/8}$,

$$\psi(x) = \int_{4c^2(g_1-g_2)}^{4c^2(g_1+g_2)} \Phi(E)u_1(x;E)\rho(E)\mathrm{d}E$$
$$+ \int_{4c^2(g_1+g_2)}^{\infty} \Phi_i(E)\rho_{ij}(E)T_j(x;E)\mathrm{d}E + \sum_{n=0}^{n_{\max}} Q_n^2\Phi_n(E)u_1(x;E_n),$$

$$\Phi(E) = \int_{\mathbb{R}} u_1(x;E)\psi(x)\mathrm{d}x,\ 4c^2(g_1-g_2) \le E < 4c^2(g_1+g_2),$$

$$\Phi_i(E) = \int_{\mathbb{R}} T_i(x;E)\psi(x)\mathrm{d}x,\ E \ge 4c^2(g_1+g_2),\ i = 1, 2,$$

$$\Phi_n(E) = \int_{\mathbb{R}} u_1(x;E_n)\psi(x)\mathrm{d}x,\ n = 0, 1, \ldots, n_{\max},$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2\mathrm{d}x = \int_{4c^2(g_1-g_2)}^{4c^2(g_1+g_2)} |\Phi(E)|^2\rho(E)\mathrm{d}E u_1(x;E)$$
$$+ \int_{4c^2(g_1+g_2)}^{\infty} \overline{\Phi_i(E)}\rho_{ij}(E)\Phi_j(E)\mathrm{d}E$$
$$+ \sum_{n=0}^{n_{\max}} Q_n^2|\Phi_n(E)|^2.$$

The spectrum is twofold for $E \ge 4c^2(g_1+g_2)$ and is simple for $E<4c^2(g_1+g_2)$ (only the combination $e_kT_k = u_1$ enters the inversion formulas), in complete agreement with physical considerations.

8.9 ESP IX

In this case

$$V(x) = 4c^2[g_1\coth^2(cx) + g_2\coth(cx)],\quad x \in \mathbb{R}_+, \tag{8.126}$$

and the corresponding Schrödinger equation is

$$\psi'' - 4c^2[g_1\coth^2(cx) + g_2\coth(cx)]\psi + W\psi = 0. \tag{8.127}$$

It is sufficient to consider only the case $c > 0$ without loss of generality.

The potential (8.126) is known as the *Eckart potential*; see [52]. This potential is used to describe effects involving all sorts of barrier penetration: tunneling, molecular barrier permeability, and so on [29].

Introducing a new variable z and new functions $\phi_{\xi_\mu,\xi_\nu}(z)$, instead of x and $\psi(x)$ in (8.127),

$$z = 1 - \mathrm{e}^{-2cx},\ z \in [0, 1),$$
$$\psi(x) = z^{1/2+\xi_\mu \mu}(1-z)^{\xi_\nu \nu}\phi_{\xi_\mu,\xi_\nu}(z),\ \xi_\mu, \xi_\nu = \pm 1,$$

where

$$\mu = \begin{cases} 2\sqrt{g_1 + 1/16},\ g_1 \geq -1/16 \\ i\varkappa,\ \varkappa = 2\sqrt{|g_1| - 1/16},\ g_1 < -1/16 \end{cases},\ \mu^2 = 4g_1 + 1/4,$$
$$\nu = \sqrt{g_1 + g_2 - w} = \sqrt{\rho_1}\mathrm{e}^{-i\varphi_1/2},\ g_1 + g_2 - w = \rho_1 \mathrm{e}^{-i\varphi_1},$$
$$\lambda = \sqrt{g_1 - g_2 - w} = \sqrt{\rho_2}\mathrm{e}^{-i\varphi_2/2},\ g_1 - g_2 - w = \rho_2 \mathrm{e}^{-i\varphi_2},$$
$$w = W/(4c^2) = a + ib,\ b \geq 0,\ 0 \leq \varphi_{1,2} \leq \pi,$$

we obtain equations for the new functions,

$$z(1-z)d_z^2\phi_{\xi_\mu}(z) + [\gamma_{\xi_\mu} - (1 + \alpha_{\xi_\mu} + \beta_{\xi_\mu})z]d_z\phi_{\xi_\mu}(z) - \alpha_{\xi_\mu}\beta_{\xi_\mu}\phi_{\xi_\mu}(z) = 0,$$
$$\alpha_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu + \lambda,\ \beta_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu - \lambda,\ \gamma_{\xi_\mu} = 1 + 2\xi_\mu\mu.$$

Solutions of these equations are the hypergeometric functions $F(\alpha, \beta; \gamma; z)$; see [1, 20, 81].

Introducing a new variable $u = 1 - z$ and a new function $\phi_{\xi_\nu}(u)$ instead of x and $\psi(x)$ in (8.127),

$$\psi(x) = (1-u)^{1/2+\mu}u^{\xi_\nu \nu}\phi_{\xi_\nu}(u),$$

we obtain an equation for $\phi_{\xi_\nu}(u)$,

$$u(1-u)d_u^2\phi_{\xi_\nu}(u) + [\gamma'_{\xi_\nu} - (1 + \alpha_{\xi_\nu} + \beta_{\xi_\nu})u]d_u\phi_{\xi_\nu}(u) - \alpha_{\xi_\nu}\beta_{\xi_\nu}\phi_{\xi_\nu}(u) = 0,$$
$$\alpha_{\xi_\nu} = 1/2 + \mu + \xi_\nu\nu + \lambda,\ \beta_{\xi_\nu} = 1/2 + \mu + \xi_\nu\nu - \lambda,\ \gamma'_{\xi_\nu} = 1 + 2\xi_\nu\nu.$$

In what follows, we will use four solutions of (8.127):

$$\begin{aligned} u_1(x; W) &= z^{1/2+\mu}(1-z)^\nu F(\alpha_1, \beta_1; \gamma_1; z) = u_1(x; W)|_{\nu \to -\nu} \\ u_2(x; W) &= z^{1/2-\mu}(1-z)^\nu F(\alpha_2, \beta_2; \gamma_2; z) = u_2(x; W)|_{\nu \to -\nu} \\ &= u_1(x; W)|_{\mu \to -\mu}, \\ V_1(x; W) &= z^{1/2+\mu}(1-z)^\nu F(\alpha_1, \beta_1; \gamma_3; 1-z) = V_1(x; W)|_{\mu \to -\mu}, \\ V_2(x; W) &= z^{1/2+\mu}(1-z)^{-\nu} F(\alpha_4, \beta_4; \gamma_4; 1-z) = V_2(x; W)|_{\mu \to -\mu} \\ &= V_1(x; W)|_{\nu \to -\nu}, \end{aligned} \tag{8.128}$$

where

$$\alpha_1 = \alpha_{+,+} = 1/2 + \mu + \nu + \lambda,\ \beta_1 = \beta_{+,+} = 1/2 + \mu + \nu - \lambda,$$
$$\alpha_2 = \alpha_{-,+} = 1/2 - \mu + \nu + \lambda,\ \beta_2 = \beta_{-,+} = 1/2 - \mu + \nu - \lambda,$$
$$\alpha_4 = \alpha_{+,-} = 1/2 + \mu - \nu + \lambda,\ \beta_4 = \beta_{+,-} = 1/2 + \mu - \nu - \lambda,$$
$$\gamma_1 = \gamma_+ = 1 + 2\mu,\ \gamma_2 = \gamma_- = 1 - 2\mu,\ \gamma_3 = \gamma'_+ = 1 + 2\nu,\ \gamma_4 = \gamma'_- = 1 - 2\nu.$$

There are relations between the introduced solutions:

$$u_1 = \frac{\Gamma(\gamma_1)\Gamma(-2\nu)}{\Gamma(\alpha_4)\Gamma(\beta_4)}V_1 + \frac{\Gamma(\gamma_1)\Gamma(2\nu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}V_2,$$
$$V_1 = \frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}u_1 + \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_2.$$

We note that the functions u_k, $k = 1, 2$, are entire in W; in particular, u_k, $k = 1, 2$, are real entire in W for $g_1 \geq -1/16$ ($\mu \geq 0$), and $u_2\,(x; E) = \overline{u_1\,(x; E)}$ for $g_1 < -1/16$ ($\mu = -i\varkappa$).

The asymptotic behavior of special functions in solutions (8.128) is well known, see [1, 20], so that we can obtain their asymptotics.

As $x \to 0$, $z = 2cx\tilde{O}(x) \to 0$, we have

$$u_1(x; W) = z^{1/2+\mu}\tilde{O}(z) = (2cx)^{1/2+\mu}\tilde{O}(x),$$
$$u_2(x; W) = z^{1/2-\mu}\tilde{O}(z) = (2cx)^{1/2-\mu}\tilde{O}(x),$$
$$\operatorname{Im} W \geq 0:\ V_1(x; W) =$$
$$\begin{cases} \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}(cx)^{1/2-\mu}\tilde{O}(x),\ g_1 \geq 3/16, \\ \left[\frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}(2cx)^{1/2+\mu} + \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}(2cx)^{1/2-\mu}\right]\tilde{O}(x),\ g_1 < 3/16. \end{cases} \tag{8.129}$$

As $x \to \infty$, $1 - z = \mathrm{e}^{-2cx} \to 0$, $z \to 1$, $\operatorname{Im} W > 0$, we have

$$u_1(x; W) = \frac{\Gamma(\gamma_1)\Gamma(2\nu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}\mathrm{e}^{2\nu cx}\tilde{O}(\mathrm{e}^{-2cx}),$$
$$V_1(x; W) = \mathrm{e}^{-2\nu cx}\tilde{O}\left(\mathrm{e}^{-2cx}\right).$$

The above asymptotics allow us to obtain

$$\operatorname{Wr}(u_1, u_2) = -4\mu c,\ \operatorname{Wr}(u_1, V_1) = -\frac{2c\Gamma(\gamma_1)\Gamma(\gamma_3)}{\Gamma(\alpha_1)\Gamma(\beta_1)} = -\omega(W).$$

Thus, solutions u_1 and V_1 are linearly independent and form a fundamental set of solutions of (8.127) for $\operatorname{Im} W \neq 0$

One can see that for $g_1 < 3/16$ ($\mu < 1$), the function $V_1(x; W)$ is square-integrable at the origin (moreover, any solution is square-integrable at the origin), and for $g_1 \geq 3/16$ ($\mu \geq 1$), it is not. Thus, for $g_1 \geq 3/16$, (8.127) has no square-integrable solutions (for $\operatorname{Im} W \neq 0$), so that the deficiency indices of the initial symmetric operator $\hat{H}$ are zero. For $g_1 < 3/16$, such an equation has only one square-integrable solution, $V_1(x; W)$, so that the deficiency indices are $m_\pm = 1$.

As usual, starting with the s.a. differential operation $\check{H}$ with the potential (8.126), we construct the initial symmetric operator $\hat{H}$ defined on the domain $\mathcal{D}(\mathbb{R}_+)$. Its adjoint $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$.

8.9.1 Range 1

In this range, we have

$$g_1 \geq 3/16 \ (\mu \geq 1).$$

Let us study the asymptotic behavior of the functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$ as $x \to 0$ and as $x \to \infty$. Such functions can be considered square-integrable solutions of the equation

$$\check{H}\psi_* = \eta \in L^2(\mathbb{R}_+). \tag{8.130}$$

Its general solution has the form

$$\begin{aligned}\psi_*(x) = {} & a_1 u_1(x;0) + a_2 V_1(x;0) \\ & + \omega^{-1}(0)\left[u_1(x;0)\int_x^\infty V_1(y;0) + \int_0^x V_1(x;0)u_1(y;0)\right]\eta(y)\mathrm{d}y\end{aligned}$$

(one can verify that $\gamma_1, \gamma_2, \alpha_1, \beta_1 \neq -n$, $n \in \mathbb{Z}_+$, so that $\omega(0) \neq 0$ and $u_1(x;0)$ and $V_1(x;0)$ are independent). The condition $\psi_* \in L^2(\mathbb{R}_+)$ implies $a_1 = a_2 = 0$. Because the potential (8.126) is bounded at infinity, we have $[\psi_*, \psi_*]|^\infty = 0$ according to Theorem 7.1.

The asymptotics of the functions $\psi_*(x)$ and $\psi_*'(x)$ as $x \to 0$ can be found by estimation of integral summands with the help of the Cauchy–Schwarz inequality,

$$\psi_*(x) = \begin{cases} O(x^{3/2}), & g_1 > 3/16, \\ O(x^{3/2}\sqrt{\ln x}), & g_1 = 3/16, \end{cases}$$

$$\psi_*'(x) = \begin{cases} O(x^{1/2}), & g_1 > 3/16, \\ O(x^{1/2}\sqrt{\ln x}), & g_1 = 3/16. \end{cases}$$

Calculating the asymmetry form, we obtain $\Delta_{H^+}(\psi_*) = 0$, $\forall \psi_* \in D^*_{\check{H}}(\mathbb{R})$. This result implies that the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

To construct the Green's function of the operator $\hat{H}_1$, we consider, following Sect. 5.3.2, the general solution of the inhomogeneous equation

$$(\check{H} - W)\psi = \eta \in L^2(\mathbb{R}_+),\ \operatorname{Im} W > 0.$$

Such a solution has the form

$$\psi(x) = a_1 u_1(x;W) + a_2 V_1(x;W) + I(x;W),\ I(x;W) = \omega^{-1}(W)$$
$$\times \left[u_1(x;W) \int_x^\infty V_1(y;W)\eta(y)\mathrm{d}y + V_1(x;W)\int_0^x u_1(y;W)\eta(y)\mathrm{d}y \right]. \quad (8.131)$$

With the help of the Cauchy–Schwarz inequality, we can estimate that both terms in square brackets are bounded as $x \to \infty$, which implies $a_1 = 0$ for $\psi \in L^2(\mathbb{R}_+)$. As $x \to 0$, we obtain that $I(x) \sim O(x^{3/2})$ (with logarithmic accuracy for $g_1 = 3/16$) and $V_1(x;W)$ is not square-integrable at the origin. Then $\psi \in L^2(\mathbb{R}_+)$ implies $a_2 = 0$.

Thus, the Green's function of the operator $\hat{H}_1$ has the form

$$G(x, y; W) = \begin{cases} V_1(x;W)u_1(y;W),\ x > y, \\ u_1(x;W)V_1(y;W),\ x < y, \end{cases}$$

so that

$$M(x_0;W) = G(x_0 - 0, x_0 + 0; W) = \omega^{-1}(W)u_1(x_0;W)V_1(x_0;W).$$

For $m - 1 < 2\mu < m + 1$, $m \geq 2$, we represent $V_1(x;W)$ as

$$V_1(x;W) = A_m(W)u_1(x;W) + \frac{\omega(W)}{4\mu c}V_{(m)}(x;W),$$
$$A_m(W) = \frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)} + a_m(W)\frac{\Gamma(\gamma_3)\Gamma(2\mu)\Gamma(\gamma_2)}{\Gamma(\alpha_1)\Gamma(\beta_1)},$$
$$V_{(m)}(x;W) = u_2(x;W) - a_m(W)\Gamma(\gamma_2)u_1(x;W),$$
$$a_m(W) = \left.\frac{\Gamma(\alpha_2 + m)\Gamma(\beta_2 + m)}{m!\Gamma(\alpha_2)\Gamma(\beta_2)}\right|_{2\mu = m}.$$

Using the second relation (8.116), one can verify that all the functions $V_{(m)}(x;W)$ exist for any W and for $m - 1 < 2\mu < m + 1$. Note that $a_m(W)$ are polynomials in ν^2 and λ^2, and therefore in W, with real coefficients, so that $a_m(E)$ are real and $V_{(m)}(x;W)$ are real entire functions in W. One can also verify that $A_m(W)$ exist for any W and for $m - 1 < 2\mu < m + 1$, and $A_m(E)$ are real. In addition, $V_{(m)}(x;W)$ are solutions of (8.127) and

$$\mathrm{Wr}(u_1, V_{(m)}) = -4\mu c,\ V_{(m)}(x;W) = (cx)^{1/2-\mu}\tilde{O}(x),\ x \to 0.$$

Let us consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_1(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ ($\tilde{U} = V_{(m)}$), and therefore the spectrum of $\hat{H}_1$ is simple.

Following Chap. 5, we obtain the derivative of the spectral function,

$$\sigma'(E) = \operatorname{Im} \left. \frac{V_1(x_0; W)}{\pi\omega(W)u_1(x_0; W)} \right|_{W=E+i0} = \operatorname{Im} B(E + i0),$$
$$B(W) = \frac{A_m(W)}{\pi\omega(W)},\ m - 1 < 2\mu < m + 1. \tag{8.132}$$

Since $B(W)$ is an analytic function of μ, the value of $\operatorname{Im} B(W)$ at the point $\mu = m/2$ can be found as a limit $\mu \to m/2$. For $\mu \neq m/2$, the quantity $\sigma'(E)$ is essentially simplified:

$$\sigma'(E) = -\frac{\Gamma(\gamma_2) \operatorname{Im} \Omega^{-1}(E + i0)}{4\pi c\mu\Gamma(\gamma_1)},\ \Omega^{-1}(W) = \frac{\Gamma(\alpha_1)\Gamma(\beta_1)}{\Gamma(\alpha_2)\Gamma(\beta_2)}.$$

For $E \geq 4c^2\,(g_1 + g_2)$ and $\nu = -ip$, $p = \sqrt{E/(4c^2) - g_1 - g_2} \geq 0$, we have

$$\sigma'(E) = \rho^2(E),\ \rho(E) = \frac{|\Gamma(\alpha_1)\Gamma(\beta_1)|}{2\pi\Gamma(\gamma_1)}\sqrt{\frac{\sin h(2\pi p)}{c}}. \tag{8.133}$$

One can see that $0 < \sigma'(E) < \infty$ for $p > 0$. If $\sqrt{-2g_2} \neq 1/2 + \mu + n$, $n \in \mathbb{Z}_+$, then $\sigma'(E) = 0$ for $p = 0$. If $\sqrt{-2g_2} = 1/2+\mu+n$, then $\sigma'(E)$ has an integrable singularity of the type $\sim p^{-1}$, which means the absence of discrete levels for $p = 0$. This matches the fact that (8.127) has no square-integrable solutions for $E/4c^2 = g_1 + g_2$. Thus, all points of the semiaxis $E \geq 4c^2(g_1 + g_2)$ belong to the continuous spectrum of $\hat{H}_1$.

For $E < 4c^2\,(g_1 + g_2)$ and $\nu = \sqrt{g_1 + g_2 - E/4c^2} > 0$, the function $\Omega^{-1}(E)$ is real for any E where $\Omega(E) \neq 0$. That is why only points E_n obeying the equation

$$\Omega(E_n) = 0 \Longrightarrow \beta_1 + n = 0,\ n \in \mathbb{Z}_+,$$

can provide nonzero contributions to $\sigma'(E)$. Thus, in this case, we obtain

$$\sigma'(E) = \sum_{n=0}^{n_{1\max}} Q_n^2 \delta(E - E_n),$$

$$Q_n = \sqrt{\frac{4c\nu_n\lambda_n \Gamma(\gamma_1 + n)\Gamma(\gamma_1 + 2\nu_n + n)}{n!\Gamma^2(\gamma_1)\Gamma(1 + 2\nu_n + n)\,(\lambda_n - \nu_n)}},$$

$$\lambda_n = \sqrt{g_1 - g_2 - E_n/4c^2} > \nu_n = \sqrt{g_1 + g_2 - E_n/4c^2}, \tag{8.134}$$

where E_n are solutions of the equation

$$1/2 + \mu + \sqrt{g_1 + g_2 - E_n/4c^2} - \sqrt{g_1 - g_2 - E_n/4c^2} = -n. \tag{8.135}$$

Equation (8.135) has solutions E_n only if $g_2 < 0$ and $2|g_2| > (1/2 + \mu)^2$. They are

$$E_n = 4c^2 g_1 - \left(\frac{2cg_2}{1/2 + \mu + n}\right)^2 - c^2(1/2 + \mu + n)^2. \tag{8.136}$$

The number of all discrete levels is equal to $n_{\max} + 1$,

$$n_{\max} = \begin{cases} [K]\,, \text{ for } [K] < K, \\ [K] - 1, \text{ for } [K] = K, \end{cases} \tag{8.137}$$

where $K = \sqrt{2|g_2|} - 1/2 - \mu$. At least one discrete level exists for $2|g_2| > (1/2 + \mu)^2$.

Finally, the simple spectrum of the operator $\hat{H}_1$ is given by

$$\text{spec } \hat{H}_1 = [g_1 + g_2, \infty) \cup \{E_n,\ n = 0, 1, \dots, n_{\max}\}.$$

The (generalized) eigenfunctions

$$U(x; E) = \rho(E)u_1(x; E),\ E \geq 4c^2(g_1 + g_2),$$

$$U_n(x) = Q_n u_1(x; E_n),\ E_n < 4c^2(g_1 + g_2),\ n = 0, 1, \dots, n_{\max},$$

of the operator $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

8.9.2 Range 2

In this range, we have

$$3/16 > g_1 > -1/16 \ (1 > \mu > 0).$$

In this range, it is convenient to introduce a new solution $u_3(x;W)$ of (8.127),

$$
\begin{aligned}
u_3(x;W) &= u_2(x;W) + \frac{2g_2\Gamma(-2\mu)}{\Gamma(2\mu)}u_1(x;W),\\
V_1(x;W) &= [\tilde{A}_1(W) - \tilde{B}_1(W)]u_1(x;W) + \tilde{C}_1(W)u_3(x;W),\\
\tilde{A}_1(W) &= \frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)},\ \tilde{C}_1(W) = \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)} = \frac{\omega(W)}{4\mu c},\\
\tilde{B}_1(W) &= \frac{2g_2\Gamma(-2\mu)}{\Gamma(2\mu)}\tilde{C}_1(W) = \frac{2g_2\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}.
\end{aligned}
$$

The solution $u_3(x;W)$ is real entire in W and the solutions u_1, u_3, and V_1 have the following asymptotic behavior as $x \to 0$:

$$
\begin{aligned}
u_1(x;W) &= u_{1\mathrm{as}}(x) + O(x^{3/2}),\ u_{1\mathrm{as}}(x) = (2cx)^{1/2+\mu},\\
u_3(x;W) &= u_{3\mathrm{as}}(x) + O(x^{3/2}),\\
u_{3\mathrm{as}}(x) &= (2cx)^{1/2-\mu} - 2g_2\frac{\Gamma(\gamma_2)}{\Gamma(\gamma_1)}(2cx)^{1/2+\mu} + \frac{2g_2}{\gamma_2}(2cx)^{3/2-\mu},\\
V_1(x;W) &= [\tilde{A}_1(W) - \tilde{B}_1(W)]u_{1\mathrm{as}}(x) + \tilde{C}_1(W)u_{3\mathrm{as}}(x) + O(x^{3/2}).
\end{aligned}
$$

Using the asymptotics, we obtain $\mathrm{Wr}(u_1, u_3) = -4\mu c$.

As for whether in the range under consideration, any solution of (8.127) is square-integrable at the origin, we represent the general solution of (8.130) as follows:

$$
\begin{aligned}
\psi_*(x) =& a_1u_1(x;0) + a_2u_3(x;0)\\
&+ \frac{1}{4\mu c}\int_0^x \Big[u_3(x;0)u_1(y;0) - u_1(x;0)u_3(y;0)\Big]\eta(y)\mathrm{d}y. \qquad (8.138)
\end{aligned}
$$

As in the previous section, here we have $[\psi_*, \psi_*]|^{\infty} = 0$.

The asymptotics of the functions $\psi_*(x)$ and $\psi_*'(x)$ as $x \to 0$ can be found by estimating the integral summands with the help of the Cauchy–Schwarz inequality,

$$
\begin{aligned}
\psi_*(x) &= a_1u_{1\mathrm{as}}(x) + a_2u_{3\mathrm{as}}(x) + O(x^{3/2}),\\
\psi_*'(x) &= a_1u_{1\mathrm{as}}'(x) + a_2u_{3\mathrm{as}}'(x) + O(x^{1/2}). \qquad (8.139)
\end{aligned}
$$

Using these asymptotics, we obtain $\Delta_{H^+}(\psi_*) - 4\mu c(\overline{a_1}a_2 - \overline{a_2}a_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1\cos\zeta = a_2\sin\zeta$, $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$. Thus, in the range under consideration, there exists a family of s.a. operators $\hat{H}_{2,\zeta}$ parameterized by ζ with domains $D_{H_{2,\zeta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{2,\zeta\mathrm{as}}(x) + O(x^{3/2}),\ \psi'(x) = C\psi'_{2,\zeta\mathrm{as}}(x) + O(x^{1/2}),$$
$$\psi_{2,\zeta\mathrm{as}}(x) = u_{1\mathrm{as}}(x)\sin\zeta + u_{3\mathrm{as}}(x)\cos\zeta. \tag{8.140}$$

Therefore,

$$D_{H_{2,\zeta}} = \{\psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy } (8.140)\}.$$

Imposing the boundary conditions (8.140) on the functions (8.131) (with $a_1 = 0$) and using asymptotics (8.139), we obtain the Green's function of the Hamiltonian $\hat{H}_{2,\zeta}$,

$$G(x, y; W) = \Omega^{-1}(W)U_{2,\zeta}(x; W)U_{2,\zeta}(y; W) - \frac{1}{4\mu c}\begin{cases} \tilde{U}_{2,\zeta}(x; W)U_{2,\zeta}(y; W),\ x > y, \\ U_{2,\zeta}(x; W)\tilde{U}_{2,\zeta}(y; W),\ x < y. \end{cases} \tag{8.141}$$

Here

$$U_{2,\zeta}(x; W) = u_1(x; W)\sin\zeta + u_3(x; W)\cos\zeta,$$
$$\tilde{U}_{2,\zeta}(x; W) = u_1(x; W)\cos\zeta - u_3(x; W)\sin\zeta,$$
$$\omega_\zeta(W) = \frac{\tilde{A}_1(W) - \tilde{B}_1(W)}{\tilde{C}_1(W)}\cos\zeta - \sin\zeta,$$
$$\tilde{\omega}_\zeta(W) = \frac{\tilde{A}_1(W) - \tilde{B}_1(W)}{\tilde{C}_1(W)}\sin\zeta + \cos\zeta,\ \Omega(W) = -\frac{4\mu c\omega_\zeta(W)}{\tilde{\omega}_\zeta(W)},$$
$$4\mu c\omega^{-1}(W)V_1(x; W) = \tilde{\omega}_\zeta(W)U_{2,\zeta}(x; W) + \omega_\zeta(W)\tilde{U}_{2,\zeta}(x; W).$$

We note that $U_{2,\zeta}$ and $\tilde{U}_{2,\zeta}$ are solutions of (8.127) real entire in W, $U_{2,\zeta}$ satisfies the boundary condition (8.140), and the second summand on the right-hand side of (8.141) is real for real $W = E$.

Let us consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x U_{2,\zeta}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{2,\zeta}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{2,\zeta}$ ($\tilde{U} = \tilde{U}_{2,\zeta}$), and therefore the spectra of $D_{H_{2,\zeta}}$ are simple.

Using the Green's function, we obtain the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E+i0)$. We first consider the extension with $\zeta = \pi/2$. In this case we have $U_{2,\pi/2}(x; W) = u_1(x; W)$, and in fact, the function $\Omega^{-1}(W)$ is reduced to the function $B(W)$ given by (8.132) for $\mu \in (0, 1)$, namely, $\pi^{-1}\Omega^{-1}(W) = B(W)$. Therefore, we can use results obtained in the first range. Finally, we have for the simple spectrum of the s.a. Hamiltonian $\hat{H}_{2,\pi/2}$,

$$\mathrm{spec}\,\hat{H}_{2,\pi/2} = [g_1 + g_2, \infty) \cup \{\mathcal{E}_n,\ n = 0, 1, \ldots, n_{\max}\},$$

where the discrete spectrum points $\mathcal{E}_n$ are given by the right-hand side of (8.136) and $n_{\max}$ is given by (8.137). The set of (generalized) eigenfunctions

$$U_E(x) = \rho(E)U_{2,\pi/2}(x;E),\ E \geq 4c^2(g_1+g_2),$$
$$U_n(x) = Q_n U_{2,\pi/2}(x;\mathcal{E}_n),\ n = 0,1,\ldots,n_{\max},$$

of $\hat{H}_{2,\pi/2}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. Here $\rho(E)$ and Q_n are given by (8.133) and (8.134). For the case $\zeta = -\pi/2$, we obtain the same results.

Considering extensions with $|\zeta| < \pi/2$, we represent $\sigma'(E)$ as

$$\sigma'(E) = \left(4\pi\mu c\cos^2\zeta\right)^{-1}\operatorname{Im} f_\zeta^{-1}(E+i0),\ f_\zeta(W) = f(W) + \tan\zeta,$$
$$f(W) = \frac{\tilde{A}_1(W) - \tilde{B}_1(W)}{\tilde{C}_1(W)} = \frac{\Gamma(\gamma_2)}{\Gamma(\gamma_1)}\left[\frac{\Gamma(\alpha_1)\Gamma(\beta_1)}{\Gamma(\alpha_2)\Gamma(\beta_2)} - 2g_2\right].$$

For $E \geq 4c^2(g_1+g_2)$, $\nu = -ip$, $p = \sqrt{E/(4c^2) - g_1 - g_2} \geq 0$, and $f(E) = A(E) - iB(E)$, we have $\sigma'(E) = \rho^2(E) > 0$, where

$$\rho(E) = \frac{|\Gamma(\alpha_2)\Gamma(\beta_2)|\sqrt{c^{-1}\sin h(2\pi p)}}{2\pi\Gamma(\gamma_1)|F(E)|\cos\zeta},\ |f_\zeta(E)|^2 = [A(E) - \tan\zeta]^2 + B^2(E),$$
$$A(E) = \frac{2\pi\mu}{\sin(2\pi\mu)\Gamma^2(\gamma_1)}$$
$$\times\left(\frac{1}{2\pi^2}|\Gamma(\alpha_1)\Gamma(\beta_1)|^2[\cos(2\pi\mu)\cos h(2\pi p) + \cos(2\pi\lambda)] - 2g_2\right),$$
$$B(E) = \frac{\mu|\Gamma(\alpha_1)\Gamma(\beta_1)|^2}{\pi\Gamma^2(\gamma_1)}\sin h(2\pi p).$$

For $E > 4c^2(g_1+g_2)$, the function $\rho^2(E)$ is finite. For $E = 4c^2(g_1+g_2)$, the function $\rho^2(E)$ is finite if $\tan\zeta \neq A(4c^2(g_1+g_2))$, and if $\tan\zeta = A(4c^2(g_1+g_2))$, we have $\rho^2(E) \longrightarrow O(1/p)$ as $E \to 4c^2(g_1+g_2)$, so that all $E \geq 4c^2(g_1+g_2)$ belong to the simple continuous spectrum of $\hat{H}_{2,\zeta}$.

For $E < 4c^2(g_1+g_2)$, $\nu = \sqrt{g_1+g_2-E/4c^2} > 0$, the function $f_\zeta(E)$ is real, so that $\sigma'(E)$ differs from zero only at the points $E_n(\zeta)$ for which $f_\zeta(E_n(\zeta)) = 0$. Therefore,

$$\sigma'(E) = \textstyle\sum_{n\in\Lambda} Q_n^2\delta(E - E_n(\zeta)),\ Q_n = \left[-4\mu c f_\zeta'(E_n(\zeta))\right]^{-1/2},$$
$$f_\zeta'(E_n(\zeta)) < 0,$$

where $\Lambda = -1,0,1,\ldots,n_{\max}$; see below.

Finally, the simple spectrum of $\hat{H}_{2,\zeta}$ is given by

$$\operatorname{spec} \hat{H}_{2,\zeta} = [g_1 + g_2, \infty) \cup \{E_n(\zeta),\ n \in \Lambda\},\ E_n(\zeta) < 4c^2(g_1 + g_2).$$

The set of (generalized) eigenfunctions

$$U_E(x) = \rho(E)U_{2,\zeta}(x; E),\ E \geq 4c^2(g_1 + g_2),$$
$$U_n(x) = Q_n U_{2,\zeta}(x; E_n(\zeta)),\ n = -1, 0, 1, \dots, n_{\max},$$

of $\hat{H}_{2,\zeta}$ forms a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

Let us rewrite the spectrum equation as $f(E_n(\zeta)) = -\tan\zeta$, taking into account that

$$\partial_\zeta E_n(\zeta) = -\left[f'(E_n(\zeta))\cos^2\zeta\right]^{-1} > 0,\ f(E) \overset{E\to-\infty}{\longrightarrow} \infty,$$

and

(1) For $2g_2 \geq -(1/2+\mu)^2$: $f(E)$ is smooth for $E \in (-\infty, 4c^2(g_1+g_2)-0)$;
(2) For $2g_2 = -(1/2+\mu+k)^2$, $k \in \mathbb{N}$: $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \dots, k-1$, and $f(4c^2(g_1+g_2)-0) = -\infty$;
(3) For $-(1/2+\mu+k+1)^2 < 2g_2 < -(1/2+\mu+k)^2$, $k \in \mathbb{Z}_+$: we have $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \dots, k$.

Then some remarks to the spectrum structure can be made: In the region (1): there are no discrete negative levels ($n_{\max} = -2$) for extensions with $\zeta \in [\zeta_{(0)}, \pi/2))$, where $\zeta_{(0)} = \arctan f(4c^2(g_1+g_2))$. For any $\zeta \in (-\pi/2, \zeta_{(0)})$, there exists one discrete level $E_{-1}(\zeta)$ ($n_{\max} = -1$), which increases monotonically from $\mathcal{E}_{-1}$ to $4c^2(g_1+g_2)-0$ as ζ goes from $-\pi/2+0$ to $\zeta_{(0)}-0$ (we set $\mathcal{E}_{-1} = -\infty$).

In the region (2): For any extension with $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n = -1, 0, \dots, k-1$, there exists one discrete level $E_n(\zeta)$ ($n_{\max} = k-1$), which increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ζ goes from $-\pi/2+0$ to $\pi/2-0$.

In the region (3): For any extension with $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n = -1, 0, \dots, k-1$, there exists one discrete level $E_n(\zeta)$ ($n_{\max} = k-1$), which increases monotonically from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ζ goes from $-\pi/2+0$ to $\pi/2-0$. For any extension with $\zeta \in [\zeta_{(0)}, \pi/2)$, there are no other discrete levels ($n_{\max} = k-1$). For any $\zeta \in (-\pi/2, \zeta_{(0)})$, there is one discrete level $E_k(\zeta) \in (\mathcal{E}_k, 4c^2(g_1+g_2))$ ($n_{\max} = k$) which increases monotonically from $\mathcal{E}_k + 0$ to $4c^2(g_1+g_2)-0$ as ζ goes from $-\pi/2+0$ to $\zeta_{(0)}-0$.

Note that the relation

$$\lim_{\zeta\to\pi/2} E_{n-1}(\zeta) = \lim_{\zeta\to-\pi/2} E_n(\zeta) = \mathcal{E}_n$$

holds if the level $E_n(\zeta)$ exists.

We stress that more explicit equations for the spectral function and the discrete spectrum can be obtained for the extension with

$$\zeta = \arctan\left[2g_2\Gamma(\gamma_2)\Gamma^{-1}(\gamma_1)\right].$$

8.9.3 Range 3

In this range, we have

$$g_1 = -1/16 \; (\mu = 0).$$

Here, we use the following solutions of (8.127),

$$\begin{aligned}
u_1(x;W) &= z^{1/4}(1-z)^\nu F(\alpha,\beta;1;z) = u_1(x;W)|_{\nu\to-\nu}\,,\\
u_4(x;W) &= \frac{\partial}{\partial\mu}\, u_1(x;W)|_{\mu\neq 0}\Big|_{\mu=0;\ \nu,\lambda \text{ are fixed}} = z^{1/4}(1-z)^\nu \ln z F(\alpha,\beta;1;z)\\
&\quad + z^{1/4}(1-z)^\nu \frac{\partial}{\partial\mu} F(\alpha_1,\beta_1;\gamma_1;z)|_{\mu\neq 0}\Big|_{\mu=0;\ \nu,\lambda \text{ are fixed}}\\
&= u_4(x;W)|_{\nu\to-\nu},\\
V_1(x;W) &= z^{1/4}(1-z)^\nu F(\alpha,\beta;\gamma;1-z),\ \alpha=\alpha_+,\ \alpha_\pm = 1/2\pm\nu+\lambda,\\
&\quad \beta=\beta_+,\ \beta_\pm = 1/2\pm\nu-\lambda,\ \gamma=\gamma_+,\ \gamma_\pm = 1\pm 2\nu.
\end{aligned}$$

The solutions $u_1(x;W)$ and $u_4(x;W)$ are real entire in W. The following relations hold:

$$\begin{aligned}
V_1(x;W) &= -\frac{\partial}{\partial\mu}\left[\frac{\Gamma(\gamma_3)\Gamma(\gamma_2)}{\Gamma(\alpha_2)\Gamma(\beta_2)} u_1(x;W)\right]_{\mu=0;\ \nu,\lambda \text{ are fixed}}\\
&= j(W)\,\Gamma(\gamma) u_1(x;W) - \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} u_4(x;W)\,,\\
j(W) &= \frac{\partial}{\partial\mu}\left[\frac{\Gamma(\gamma_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)}\right]_{\mu=0;\ \nu,\lambda \text{ are fixed}} = -\frac{2\mathbf{C}+\psi(\alpha)+\psi(\beta)}{\Gamma(\alpha)\Gamma(\beta)}.
\end{aligned}$$

Below, we list some asymptotics of the introduced functions as $x\to 0$ and $x\to\infty$; see [1, 20, 81].

For $x\to 0$, $z = 2cx\tilde{O}(x)\to 0$, we have

$$\begin{aligned}
u_1(x;W) &= (2cx)^{1/2}\tilde{O}(x),\\
u_4(x;W) &= (2cx)^{1/2}\ln(2cx)\tilde{O}(x),\\
V_1(x;W) &= (2cx)^{1/2}\left[j(W)\,\Gamma(\gamma) - \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\ln(2cx)\right]\tilde{O}(x).
\end{aligned} \tag{8.142}$$

For $x \to \infty$, $1 - z = \mathrm{e}^{-2cx} \to 0$, $z \to 1$, $\operatorname{Im} W > 0$, we have

$$u_1(x; W) = \frac{\Gamma(2\nu)}{\Gamma(\alpha)\Gamma(\beta)} \mathrm{e}^{2\nu cx} \tilde{O}(\mathrm{e}^{-2cx}),$$
$$V_1(x; W) = \mathrm{e}^{-2\nu cx} \tilde{O}(\mathrm{e}^{-2cx}).$$

Regarding

$$\mathrm{Wr}\,(u_1, u_4) = 2c,\ \mathrm{Wr}\,(u_1, V_1) = -\frac{2c\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} = -\omega(W),$$

solutions u_1 and V_1 are linearly independent and form a fundamental set of solutions of (8.127) for $\operatorname{Im} W \neq 0$ and $W = 0$.

Because any solution is square-integrable at the origin in the range under consideration, it is convenient to use the general solution of (8.130) in the form (8.138) with the substitutions $u_3/4\mu c \to -u_4/2c$ and $a_2 u_3 \to -a_2 u_4$.

As in previous ranges, we have $[\psi_*, \psi_*]|^{\infty} = 0$ for functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$. Their asymptotics as $x \to 0$ are

$$\psi_*(x) = a_1 u_{1\mathrm{as}}(x) + a_2 u_{4\mathrm{as}}(x) + O(x^{3/2}),$$
$$\psi'_*(x) = a_1 u'_{1\mathrm{as}}(x) + a_2 u'_{4\mathrm{as}}(x) + O(x^{1/2}),$$
$$u_{1\mathrm{as}}(x) = (2cx)^{1/2},\ u_{4\mathrm{as}}(x) = (2cx)^{1/2} \ln(2cx).$$

Using these asymptotics, we obtain $\Delta_{H^+}(\psi_*) = 2c(\overline{a_1} a_2 - \overline{a_2} a_1)$, which means that deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1 \cos\zeta = a_2 \sin\zeta$, $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$. Thus, in the range under consideration, there exists a family of s.a. operators $\hat{H}_{3,\zeta}$ parameterized by ζ with domains $D_{H_{3,\zeta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{3\mathrm{as}}(x) + O\left(x^{3/2}\ln x\right),\ \psi'(x) = C\psi'_{3\mathrm{as}}(x) + O\left(x^{1/2}\ln x\right),$$
$$\psi_{3\mathrm{as}}(x) = u_{1\mathrm{as}}(x)\sin\zeta + u_{4\mathrm{as}}(x)\cos\zeta. \tag{8.143}$$

Therefore,

$$D_{H_{3,\zeta}} = \left\{\psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy (8.143)}\right\}.$$

Imposing the boundary conditions (8.143) on the functions (8.131) (with $a_1 = 0$) and using the asymptotics (8.142), we obtain the Green's function of the Hamiltonian $\hat{H}_{3,\zeta}$,

$$G(x, y; W) = \Omega^{-1}(W) U_{3,\zeta}(x; W) U_{3,\zeta}(y; W) + \frac{1}{2c}\begin{cases} \tilde{U}_{3,\zeta}(x; W) U_{3,\zeta}(y; W),\ x > y, \\ U_{3,\zeta}(x; W)\tilde{U}_{3,\zeta}(y; W),\ x < y. \end{cases} \tag{8.144}$$

Here

$$\begin{aligned}
U_{3,\zeta}(x;W) &= u_1(x;W)\sin\zeta + u_4(x;W)\cos\zeta,\\
\tilde{U}_{3,\zeta}(x;W) &= u_1(x;W)\cos\zeta - u_4(x;W)\sin\zeta,\\
\omega_{3,\zeta}(W) &= j(W)\Gamma(\alpha)\Gamma(\beta)\cos\zeta + \sin\zeta,\\
\tilde{\omega}_{3,\zeta}(W) &= j(W)\Gamma(\alpha)\Gamma(\beta)\sin\zeta - \cos\zeta,\ \Omega(W) = 2c\frac{\omega_{3,\zeta}(W)}{\tilde{\omega}_{3,\zeta}(W)},\\
2c\omega^{-1}(W)V_1(x;W) &= \tilde{\omega}_{3,\zeta}(W)U_{3,\zeta}(x;W) + \omega_{3,\zeta}(W)\tilde{U}_{3,\zeta}(x;W).
\end{aligned}$$

We note that $U_{3,\zeta}$ and $\tilde{U}_{3,\zeta}$ are real entire solutions in W, $U_{3,\zeta}$ satisfies the boundary condition (8.143), and the second summand on the right-hand side of (8.144) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x\, U_{3,\zeta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{3,\zeta}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{3,\zeta}$ ($\tilde{U} = \tilde{U}_{3,\zeta}$), and therefore the spectra of $D_{H_{3,\zeta}}$ are simple.

Using the Green's function, we obtain the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

We first consider the extension with $\zeta = \pi/2$. In this case, we have $U_{3,\pi/2} = u_1$ and

$$\sigma'(E) = -(2\pi c)^{-1}\,\mathrm{Im}[\psi(\alpha) + \psi(\beta)]_{W=E+i0}.$$

For $E/4c^2 \geq g_2 - 1/16$ and $\nu = -ip$, $p = \sqrt{E/(4c^2) - g_2 + 1/16} \geq 0$, we have

$$\sigma'(E) = \frac{\sin h(2\pi p).}{2c\,[\cos h(2\pi p) + \cos(2\pi\lambda)]}.$$

It follows that

$$\begin{aligned}
&0 < \sigma'(E) < \infty,\ E > 4c^2(g_2 - 1/16);\\
&\sigma'(4c^2(g_2 - 1/16)) = 0,\ g_2 \neq -(1/2+n)^2/2;\\
&\sigma'(E) = O(1/p) \text{ as } E \to 4c^2(g_2 - 1/16),\ g_2 = -(1/2+n)^2/2,
\end{aligned}$$

i.e., all points of the semiaxis $E/4c^2 \geq g_2 - 1/16$ belong to the simple continuous spectrum of $\hat{H}_{3,\pi/2}$.

For $E/(4c^2) < g_2 - 1/16$ and $\nu = \sqrt{g_2 - E/4c^2 - 1/16} > 0$, the function $[\psi(\alpha) + \psi(\beta)]_{W=E}$ is real if it is finite, so that $\sigma'(E)$ can be different from zero only at the points where $\psi(\beta)$ is infinite, i.e., at the points $\beta \in \mathbb{Z}_-$.

We obtain

$$\sigma'(E) = \sum_{n=0}^{n_{\max}} Q_n^2 \delta(E - \mathcal{E}_n), \quad Q_n = \sqrt{\frac{4c\nu_n\lambda_n}{\lambda_n - \nu_n}},$$

where the spectrum points $\mathcal{E}_n$ are solutions of the equation

$$\beta = 1/2 + \nu_n - \lambda_n = n,\ n \in \mathbb{Z}_-,$$
$$\nu_n = \sqrt{|w_n| - |g_2| - 1/16},\ \lambda_n = \sqrt{|g_2| + |w_n| - 1/16},\ \mathcal{E}_n = 4c^2 w_n.$$

Such solutions have the form

$$\nu_n = \frac{|g_2|}{n + 1/2} - \frac{n + 1/2}{2},\ \lambda_n = \frac{|g_2|}{n + 1/2} + \frac{n + 1/2}{2},$$
$$\mathcal{E}_n = -4c^2 \left[\frac{g_2^2}{(n + 1/2)^2} + \frac{(n + 1/2)^2}{4} + \frac{1}{16} \right],\quad n \in \mathbb{Z}_+ .$$

We see that for $g_2 < -1/8$, there exists at least one discrete energy level. For a given $g_2 < -1/8$, there exist $n_{\max} + 1$ discrete levels,

$$n_{\max} = \begin{cases} [K],\ K > [K], \\ [K] - 1,\ K = [K], \end{cases} \qquad K = \sqrt{2|g_2|} - 1/2.$$

Thus, the simple spectrum of $\hat{H}_{3,\pi/2}$ is given by

$$\operatorname{spec} \hat{H}_{3,\pi/2} = [g_2 - 1/16, \infty) \cup \{\mathcal{E}_n,\ n = 0, 1, \ldots, n_{\max}\}.$$

The (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} U_{3,\pi/2}(x; E),\ E \geq 4c^2(g_2 - 1/16),$$
$$U_n(x) = Q_n U_{3,\pi/2}(x; \mathcal{E}_n),\ \mathcal{E}_n < 4c^2(g_2 - 1/16),\ n = 0, 1, \ldots, n_{\max},$$

of the operator $\hat{H}_{3,\pi/2}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

For the case $\zeta = -\pi/2$, we obtain the same results.

We note that the solution of the spectral problem in the case under consideration can be obtained from the corresponding solution for $g_1 \geq 3/16$, setting there $\mu = 0$.

Let us consider extensions with $|\zeta| < \pi/2$. In this case,

$$\sigma'(E) = \left(2\pi c \cos^2 \zeta\right)^{-1} \operatorname{Im} f_\zeta^{-1}(E + i0),$$
$$f_\zeta(W) = f(W) - \tan\zeta,\ f(W) = \psi(\alpha) + \psi(\beta) + 2\mathbf{C}.$$

For $E \geq 4c^2(g_2 - 1/16)$ and $\nu = -ip$, $p = \sqrt{E/(4c^2) - g_2 + 1/16} \geq 0$, we have

$$\sigma'(E) = \frac{B(E)}{2\pi c\,[(A(E) - \tan\zeta)^2 + B^2(E)]} \geq 0,$$
$$A(E) = \operatorname{Re} f(E),\ B(E) = -\operatorname{Im} f(E) = \frac{\pi \sin h(2\pi p).}{\cos h(2\pi p) + \cos(2\pi\lambda)}.$$

The function $\sigma'(E)$ is finite and positive for any $E > 4c^2(g_2 - 1/16)$. If $\tan\zeta \neq A(4c^2(g_2 - 1/16))$, then $\sigma'(4c^2(g_2 - 1/16)) = 0$. If $\tan\zeta = A(4c^2(g_2 - 1/16))$, then $\sigma'(E) \to O(1/p)$ as $E \to 4c^2(g_2 - 1/16)$. Thus all points of the semiaxis $E/4c^2 \geq g_2 - 1/16$ belong to the simple continuous spectrum of $\hat{H}_{3,\pi/2}$.

For $E < 4c^2(g_2 - 1/16)$ and $\nu = \sqrt{g_2 - 1/16 - E/4c^2} > 0$, the function $f_\zeta(E)$ is real, so that $\sigma'(E)$ can be different from zero only at the points $E_n(\zeta)$ that satisfy the equation $f_\zeta(E_n(\zeta)) = 0$. Thus,

$$\sigma'(E) = \sum_{n\in\Lambda} Q_n^2 \delta(E - E_n(\zeta)),\ Q_n = \sqrt{-\left[2cf_\zeta'(E_n(\zeta))\right]^{-1}},$$

where $f_\zeta'(E_n) < 0$, and $\Lambda = -1, 0, 1, \ldots, n_{\max}$; see below.

Finally, we have for the simple spectrum of the operator $\hat{H}_{3,\zeta}$,

$$\operatorname{spec} \hat{H}_{3,\zeta} = [4c^2(g_1 + g_2), \infty) \cup \{E_n(\zeta),\ n \in \Lambda\}.$$

The (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}U_{3,\zeta}(x; E),\ E \geq 4c^2(g_2 - 1/16),$$
$$U_n(x) = Q_n U_{3,\zeta}(x; E_n(\zeta)),\ E < 4c^2(g_2 - 1/16),\ n \in \Lambda,$$

of the operator $\hat{H}_{3,\zeta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

Let us rewrite the equation for spectrum points $E_n(\zeta)$ in the form $f(E_n) = -\tan\zeta$, taking into account that

$$\partial_\zeta E_n(\zeta) = -\left[f'(E_n(\zeta))\cos^2\zeta\right]^{-1} > 0,\ f(E) \overset{E\to\infty}{\longrightarrow} \infty,$$

and

(1) For $g_2 \geq -1/8$: $f(E)$ is smooth on $(-\infty, 4c^2(g_2 - 1/16) - 0)$;
(2) For $2g_2 = -(1/2 + k)^2$, $k \in \mathbb{N}$: $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \ldots, k-1$, $f(4c^2(g_2 - 1/16) - 0) = -\infty$;
(3) For $-(1/2 + k + 1)^2 < 2g_2 < -(1/2 + k)^2$, $k \in \mathbb{Z}_+$: $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \ldots, k$.

Then some remarks on the spectrum structure can be made:

(1) For $\zeta \in [\zeta_{(0)}, \pi/2)$, $\zeta_{(0)})$, $\zeta_{(0)} = \arctan f(4c^2(g_2 - 1/16))$, there are no discrete levels on the negative E semiaxis ($n_{\max} = -2$). For any $\zeta \in (-\pi/2, \zeta_{(0)})$, there is one discrete eigenvalue $E_{-1}(\zeta)$ ($n_{\max} = -1$) monotonically increasing from $\mathcal{E}_{-1}$ to $4c^2(g_2 - 1/16) - 0$ as ζ goes from $-\pi/2 + 0$ to $\zeta_{(0)} - 0$ (we set $\mathcal{E}_{-1} = -\infty$).
(2) In each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n = -1, 0, \ldots, k-1$, and for any $\zeta \in (-\pi/2, \pi/2)$, there is one ($n_{\max} = k-1$) discrete eigenvalue $E_n(\zeta)$ monotonically increasing from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ζ goes from $-\pi/2 + 0$ to $\pi/2 - 0$.
(3) In each interval $(\mathcal{E}_n, \mathcal{E}_{n+1})$, $n = -1, 0, \ldots, k-1$, and for any $\zeta \in (-\pi/2, \pi/2)$, there is one discrete eigenvalue $E_n(\zeta)$ monotonically increasing from $\mathcal{E}_n + 0$ to $\mathcal{E}_{n+1} - 0$ as ζ goes from $-\pi/2 + 0$ to $\pi/2 - 0$. For any $\zeta \in [\zeta_{(0)}, \pi/2)$, there are no other discrete eigenvalues ($n_{\max} = k-1$). For any $\zeta \in (-\pi/2, \zeta_{(0)})$, there is one ($n_{\max} = k$) discrete eigenvalue $E_k(\zeta) \in (\mathcal{E}_k, 4c^2(g_2 - 1/16))$ monotonically increasing from $\mathcal{E}_k + 0$ to $4c^2(g_2 - 1/16) - 0$ as ζ goes from -$\pi/2 + 0$ to $\zeta_{(0)} - 0$.

Note that the relation

$$\lim_{\zeta \to \pi/2} E_{n-1}(\zeta) = \lim_{\zeta \to -\pi/2} E_n(\zeta) = \mathcal{E}_n$$

holds if the discrete level $E_n(\zeta)$ exists for the corresponding ζ.

8.9.4 Range 4

In this range, we have

$$g_1 < -1/16 \ (\mu = i\varkappa,\ \varkappa > 0).$$

Because any solution of (8.127) is square-integrable at the origin in the range under consideration, it is convenient to use the general solution of (8.130) in the form (8.138).

As in the previous ranges, we have $[\psi_*, \psi_*]|^{\infty} = 0$ for functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$. Their asymptotics as $x \to 0$ are

$$\psi_*(x) = a_1 u_{1\text{as}}(x) + a_2 u_{2\text{as}}(x) + O(x^{3/2}),$$
$$\psi_*'(x) = a_1 u_{1\text{as}}'(x) + a_2 u_{2\text{as}}'(x) + O(x^{1/2}),$$
$$u_{1\text{as}}(x) = (2cx)^{1/2+i\varkappa},\ u_{2\text{as}}(x) = (2cx)^{1/2-i\varkappa}.$$

Using these asymptotics, we obtain $\Delta_{H^+}(\psi_*) = 4i\varkappa c(\overline{a_1}a_1 - \overline{a_2}a_2)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1 = \mathrm{e}^{2i\theta}a_2$, $\theta \in \mathbb{S}(0, \pi)$. Thus, in the range under consideration, there exists a family of s.a. operators $\hat{H}_{4,\theta}$ parameterized by ζ with domains $D_{H_{4,\theta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\psi(x) = C\psi_{4,\theta\text{as}}(x) + O(x^{3/2}),\ \psi'(x) = C\psi_{4,\theta\text{as}}'(x) + O(x^{1/2}),$$
$$\psi_{4,\theta\text{as}}(x) = \mathrm{e}^{i\theta}u_{1\text{as}}(x) + \mathrm{e}^{-i\theta}u_{2\text{as}}(x) = \overline{\psi_{4,\theta\text{as}}(x)}. \tag{8.145}$$

Therefore,

$$D_{4,\theta} = \left\{ \psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy } (8.145) \right\}.$$

Imposing the boundary conditions (8.145) on the functions (8.131) (with $a_1 = 0$) and using the asymptotics (8.129), we obtain the Green's function of the Hamiltonian $\hat{H}_{4,\theta}$,

$$\begin{aligned} G(x, y; W) &= \Omega^{-1}(W)U_{4,\theta}(x; W)U_{4,\theta}(y; W) \\ &\quad - \frac{1}{8\varkappa c} \begin{cases} \tilde{U}_{4,\theta}(x; W)U_{4,\theta}(y; W),\ x > y, \\ U_{4,\theta}(x; W)\tilde{U}_{4,\theta}(y; W),\ x < y, \end{cases} \end{aligned} \tag{8.146}$$

Here

$$\begin{aligned} &U_{4,\theta}(x; W) = \mathrm{e}^{i\theta}u_1(x; W) + \mathrm{e}^{-i\theta}u_2(x; W), \\ &\tilde{U}_{4,\theta}(x; W) = i[\mathrm{e}^{-i\theta}u_2(x; W) - \mathrm{e}^{i\theta}u_1(x; W)], \\ &\omega_{4,\theta}(W) = \mathrm{e}^{i\theta}a(W) + \mathrm{e}^{-i\theta}b(W),\ a(W) = \frac{\Gamma(\gamma_3)\Gamma(\gamma_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)}, \\ &\tilde{\omega}_{4,\theta}(W) = \mathrm{e}^{i\theta}a(W) - \mathrm{e}^{-i\theta}b(W),\ b(W) = \frac{\Gamma(\gamma_3)\Gamma(\gamma_2)}{\Gamma(\alpha_2)\Gamma(\beta_2)}, \\ &\Omega^{-1} = 8i\varkappa c\frac{\omega_{4,\theta}(W)}{\tilde{\omega}_{4,\theta}(W)}, \\ &4\mu V_1(x; W) = \tilde{\omega}_{4,\theta}(W)U_{4\theta}(x; W) - i\omega_{4,\theta}(W)\tilde{U}_{4,\theta}(x; W). \end{aligned}$$

We note that solutions $U_{4,\theta}(x; W)$ and $\tilde{U}_{4,\theta}(x; W)$ are real entire in W, $U_{4,\theta}(x; W)$ satisfies the boundary condition (8.145), and the second summand on the right-hand side of (8.146) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x U_{4,\theta}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{4,\theta}}.$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{4,\theta}$ ($\tilde{U} = \tilde{U}_{4,\theta}$), and therefore the spectra of $D_{H_{4,\theta}}$ are simple.

Using the Green's function, we obtain the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

For $w = E/(4c^2) \geq g_1 + g_2$ and $\nu = -ip$, $p = \sqrt{E/(4c^2) - g_1 - g_2} \geq 0$, we obtain

$$\sigma'(E) = \frac{|D|^2 - 1}{8\pi\varkappa c(1 + D)(1 + \overline{D})},\quad D = \frac{\mathrm{e}^{-2i\theta}\Gamma(\gamma_2)\Gamma(\alpha_1)\Gamma(\beta_1)}{\Gamma(\gamma_1)\Gamma(\alpha_2)\Gamma(\beta_2)}.$$

One can see that $|D| > 1$ for $p > 0$,

$$|D|^2 = \frac{\cos h[2\pi(\varkappa + p)] + \cos(2\pi\lambda)}{\cos h[2\pi(\varkappa - p)] + \cos(2\pi\lambda)} > 1 \text{ for } p > 0.$$

Thus, $\sigma'(E)$ is finite and positive for $p > 0$ and can have an integrable singularity of the type $\sim p^{-1}$ as $p \to 0$ (for parameters that imply $D|_{p=0} = -1$), so that the spectra of $\hat{H}_{4,\theta}$ on the interval $\mathbb{R}_+$ are simple and continuous.

For $E/(4c^2) < g_1 + g_2$ and $\nu = \sqrt{g_1 + g_2 - E/(4c^2)} > 0$, we have

$$\begin{aligned}
&\Omega(E) = -8\varkappa c \cot\Theta(E),\ \Theta(E) = \theta_\Gamma(E) - \theta,\\
&\theta_\Gamma(E) = \frac{1}{2i}[\ln\Gamma(\gamma_2) - \ln\Gamma(\gamma_1)]\\
&\qquad\qquad + \frac{1}{2i}[\ln\Gamma(\alpha_2) + \ln\Gamma(\beta_2) - \ln\Gamma(\alpha_1) - \ln\Gamma(\beta_1)].
\end{aligned}$$

Therefore $\sigma'(E)$ can be different from zero only for energies $E_n(\theta)$ that satisfy the equation $\cot\Theta(E_n(\theta)) = 0$. Thus, we obtain

$$\begin{aligned}
&\sigma'(E) = \sum_{n\in\mathcal{N}} Q_n^2\delta(E - E_n(\theta)),\ Q_n = \left[-8\varkappa c\Theta'(E_n(\theta))\right]^{-1/2},\\
&\Theta(E_n(\theta)) = \pi/2 + \pi n,\ \Theta'(E_n(\theta)) < 0,
\end{aligned}$$

where $\mathcal{N} = n_{\min}, n_{\min} - 1, \ldots$; see below.

Finally, we have for the simple spectrum of the operator $\hat{H}_{4,\theta}$,

$$\text{spec}\ \hat{H}_{4,\theta} = [4c^2(g_1 + g_2), \infty) \cup \{E_n(\theta),\ n \in \mathcal{N}\}.$$

The (generalized) eigenfunctions

$$\begin{aligned}
&U_E(x) = \sqrt{\sigma'(E)}U_{4,\theta}(x; E),\ E \geq 4c^2(g_1 + g_2),\\
&U_n(x) = Q_n U_{4,\theta}(x; E_n(\theta)),\ E_n(\theta) < 4c^2(g_1 + g_2),\ n \in \mathcal{N},
\end{aligned}$$

of the operator $\hat{H}_{4,\theta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

Some remarks on the spectrum structure can be made: Let us rewrite the spectrum equation as follows:

$$\begin{aligned}
&\theta_\Gamma(E_n(\theta)) = \pi/2 + \pi(n + \theta/\pi),\\
&\theta'_\Gamma(E_n(\theta)) = \Theta'(E_n(\theta)) < 0,\ \partial_\theta E_n(\theta) = \left[\theta'_\Gamma(E_n(\theta))\right]^{-1} < 0. \qquad (8.147)
\end{aligned}$$

Taking into account that

$$\theta_\Gamma(E) = \varkappa \ln\sqrt{|E|} + O(1),\ E \to -\infty,$$

and $\theta_\Gamma(4c^2(g_1+g_2)) \equiv \theta_{\Gamma 0} = \pi(n_0+\delta)$ is a finite real number for any $g_1 \le -1/16$ and g_2, where $n_0 = [\theta_{\Gamma 0}/\pi]$, $0 \le \delta < 1$, we obtain the following:

(1) For a fixed n and θ, $n+\theta/\pi > n_0+\delta$, (8.147) has only one solution $E_n(\theta)$;
(2) For fixed $\theta \in (\pi\delta, \pi)$, in the energy interval $(E_{n_0}(\pi\delta){=}4c^2(g_1+g_2), E_{n_0}(\pi) = E_{n_0+1}(0))$, there is one eigenvalue $E_{n_0}(\theta)$ monotonically decreasing from $4c^2(g_1+g_2)-0$ to $E_{n_0}(\pi)+0$ as θ goes from $\pi\delta+0$ to $\pi-0$;
(3) In any energy interval $[E_n(0), E_n(\pi) = E_{n+1}(0))$, $n \ge n_0+1$, for fixed $\theta \in [0,\pi)$, there is one eigenvalue $E_n(\theta)$ monotonically decreasing from to $E_n(\pi)+0$ as θ goes from 0 to $\pi-0$;
(4) For $\theta \in (\pi\delta, \pi)$, we have $n_{\min} = n_0$;
(5) For $\theta \in [0, \pi\delta]$, we have $n_{\min} = n_0+1$;
(6) We have $E_{n+1}(0) < E_n(0)$, $\forall n$, for any $g_1 < -1/16$ and g_2, so that the spectrum is unbounded from below;
(7) For high negative energies the spectrum has the form

$$E_n = -4c^2m^2 e^{2\pi n/\varkappa}\left[1+O(1/n)\right],\ n \to \infty,$$

where $m = m(g_1, g_2, \theta)$ is a scale factor. The spectrum coincides asymptotically with the spectrum of the Calogero model (for $\alpha = g_1$).

8.10 ESP X

In this case

$$V(x) = \frac{V_1 + V_2 \cos h(2cx)}{\sin h^2(2cx)},\ x \in \mathbb{R}_+, \tag{8.148}$$

and the corresponding Schrödinger equation is

$$\psi'' - \frac{V_1 + V_2 \cos h(2cx)}{\sin h^2(2cx)}\psi + W\psi = 0, \tag{8.149}$$

It is sufficient to consider only the case $c > 0$ without loss of generality.

Let us introduce a new variable z and new functions $\phi_{\xi_\mu}(z)$, instead of x and $\psi(x)$ in (8.149),

$$z = \tan h^2(cx),\ z \in [0,1), \psi(x) = z^{1/4+\xi_\mu\mu}(1-z)^\nu \phi_{\xi_\mu}(z),\ \xi_\mu = \pm 1,$$

$$\mu = \begin{cases} \sqrt{g_1},\ g_1 \ge 0, \\ i\varkappa,\ \varkappa = \sqrt{|g_1|},\ g_1 < 0, \end{cases} \qquad g_1 = \frac{V_1 + V_2 + c^2}{16c^2},$$

$$w = W/4c^2 = |w|e^{i\varphi},\ \nu = \sqrt{-w} = \sqrt{|w|}\left(\sin\frac{\varphi}{2} - i\cos\frac{\varphi}{2}\right), 0 \le \varphi \le \pi. \tag{8.150}$$

Then we obtain an equation for $\phi_{\xi_\mu}(z)$,

$$z(1-z)d_z^2\phi_{\xi_\mu}(z) + [\gamma_{\xi_\mu} - (1+\alpha_{\xi_\mu} + \beta_{\xi_\mu})z]d_z\phi_{\xi_\mu}(z) - \alpha_{\xi_\mu}\beta_{\xi_\mu}\phi_{\xi_\mu}(z) = 0,$$

$$\alpha_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu + \lambda,\ \beta_{\xi_\mu} = 1/2 + \xi_\mu\mu + \nu - \lambda,\ \gamma_{\xi_\mu} = 1 + 2\xi_\mu\mu,$$

$$\lambda = \begin{cases} \sqrt{g_2},\ g_2 \geq 0, \\ i\kappa,\ \kappa = \sqrt{|g_2|},\ g_2 < 0, \end{cases} \qquad g_2 = \frac{V_1 - V_2 + c^2}{16c^2}. \tag{8.151}$$

Introducing the variable $u = 1 - z$ and the function $\tilde{\phi}_{\xi_\nu}(u)$ in (8.149),

$$\psi(x) = (1-u)^{1/4+\mu}u^{\xi_\nu\nu}\tilde{\phi}_{\xi_\nu}(u),\ \xi_\nu = \pm 1, \tag{8.152}$$

we obtain an equation for $\tilde{\phi}_{\xi_\nu}(u)$,

$$u(1-u)d_u^2\tilde{\phi}_{\xi_\nu}(u) + [\gamma'_{\xi_\nu} - (1+\alpha_{\xi_\nu} + \beta_{\xi_\nu})u]d_u\tilde{\phi}_{\xi_\nu}(u) - \alpha_{\xi_\nu}\beta_{\xi_\nu}\tilde{\phi}_{\xi_\nu}(u) = 0,$$

$$\alpha_{\xi_\nu} = 1/2 + \mu + \xi_\nu\nu + \lambda,\ \beta_{\xi_\nu} = 1/2 + \mu + \xi_\nu\nu - \lambda,\ \gamma'_{\xi_\nu} = 1 + 2\xi_\nu\nu. \tag{8.153}$$

The solutions of equations (8.151) and (8.153) are the hypergeometric functions $F(\alpha, \beta; \gamma; z)$; see [1, 20, 81]. The solutions $\psi(x)$ of (8.149) can be obtained from solutions of these equations by the transformations (8.150) and (8.152).

We use three solutions of (8.149),

$$u_1(x;W) = z^{1/4+\mu}(1-z)^\nu F(\alpha_1, \beta_1; \gamma_1; z) = u_1(x;W)|_{\nu\to-\nu},$$

$$u_2(x;W) = z^{1/4-\mu}(1-z)^\nu F(\alpha_2, \beta_2; \gamma_2; z) = u_2(x;W)|_{\nu\to-\nu},$$

$$V_1(x;W) = z^{1/4+\mu}(1-z)^\nu F(\alpha_1, \beta_1; \gamma_3; 1-z) = V_1(x;W)|_{\mu\to-\mu},$$

$$V_1 = \frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}u_1 + \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}u_2, \tag{8.154}$$

where

$$\alpha_{1,2} = 1/2 \pm \mu + \nu + \lambda,\ \beta_{1,2} = 1/2 \pm \mu + \nu - \lambda,$$

$$\gamma_{1,2} = 1 \pm 2\mu,\ \gamma_3 = 1 + 2\nu.$$

We note that the solutions $u_1(x;W)$ and $u_2(x;W)$ are entire in W. They are real entire in W for $g_1 \geq 0$ ($\mu \geq 0$), and $u_2(x;E) = \overline{u_1(x;E)}$ for $g_1 < 0$ ($\mu = i\varkappa$).

Using the asymptotics of special functions in solutions (8.154), see e.g. [1, 20, 81], we obtain the asymptotics of the solutions. As $x \to 0$, $z = (cx)^2\tilde{O}(x^2) \to 0$, we have

$$u_1(x;W) = z^{1/4+\mu}\tilde{O}(z) = (cx)^{1/2+2\mu}\tilde{O}(x^2),$$

$$u_2(x;W) = z^{1/4-\mu}\tilde{O}(z) = (cx)^{1/2-2\mu}\tilde{O}(x^2),\ g_1 \neq 0,$$

$$V_1(x;W) = \begin{cases} \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}(cx)^{1/2-2\mu}\tilde{O}(x^2),\ g_1 \geq 1/4, \\ \left[\frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)}(cx)^{1/2+2\mu} + \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)}(cx)^{1/2-2\mu}\right]\tilde{O}(x^2), \\ g_1 < 1/4,\ \operatorname{Im} W > 0. \end{cases} \tag{8.155}$$

As $x \to +\infty$, $1 - z = 4\mathrm{e}^{-2cx}\tilde{O}(\mathrm{e}^{-2cx}) \to 0$, $z \to 1$, $\operatorname{Im} W > 0$, we obtain

$$u_1(x;W) = \frac{\Gamma(\gamma_1)\Gamma(2\nu)}{4^\nu\Gamma(\alpha_1)\Gamma(\beta_1)}\mathrm{e}^{2\nu cx}\tilde{O}\left(\mathrm{e}^{-2cx}\right),$$
$$V_1(x;W) = 4^\nu\mathrm{e}^{-2\nu cx}\tilde{O}\left(\mathrm{e}^{-2cx}\right),$$

where we have used identity (8.117).

Regarding

$$\operatorname{Wr}(u_1,u_2) = -4\mu c,\ \operatorname{Wr}(u_1,V_1) = -\frac{2c\Gamma(\gamma_1)\Gamma(\gamma_3)}{\Gamma(\alpha_1)\Gamma(\beta_1)} = -\omega(W),$$

the solutions u_1 and V_1 form a fundamental set of solutions of (8.149) for $\operatorname{Im} W > 0$.

The initial symmetric operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}(\mathbb{R}_+)$ and its adjoint $\hat{H}^+$ on the domain $D_{H^+} = D^*_{\check{H}}(\mathbb{R}_+)$.

We note that for $g_1 \geq 1/4$, $\mu \geq 1/2$, the solution $V_1(x;W)$ is not square-integrable at the origin, but for $g_1 < 1/4$, it is (moreover, any solution of (8.149) is square-integrable at the origin). This means that for $g_1 \geq 1/4$, (8.149) has no square-integrable solutions, so that the deficiency indices of $\hat{H}$ are zero. For $g_1 < 1/4$, this equation has one square-integrable solution $V_1(x;W)$, so that the deficiency indices of $\hat{H}$ are $m_\pm = 1$.

Let us consider the inhomogeneous equation

$$(\check{H} - W)\psi = \eta \in L^2(\mathbb{R}_+),\ \operatorname{Im} W > 0.$$

Its general solution has the form

$$\psi(x) = a_1u_1(x;W) + a_2V_1(x;W) + I(x;W),\ \ I(x;W) = \omega^{-1}(W)$$
$$\times\left[u_1(x;W)\int_x^\infty V_1(y;W)\eta(y)\mathrm{d}y + V_1(x;W)\int_0^x u_1(y;W)\eta(y)\mathrm{d}y\right].$$

One can see (using the Cauchy–Schwarz inequality) that $I(x)$ is bounded as $x \to \infty$. The condition $\psi_* \in L^2(\mathbb{R}_+)$ implies $a_1 = 0$.

For $g_1 \geq 1/4$, we have $I(x) \sim O(x^{3/2})$ and $I'(x) \sim O(x^{1/2})$ as $x \to 0$ (with logarithmic accuracy for $g_1 = 1/4$), and $V_1(x;W)$ is not square-integrable at the origin. Then the condition $\psi \in L^2(\mathbb{R}_+)$ implies $a_2 = 0$.

For $g_1 < 1/4$, it is convenient to represent $\psi(x)$ as follows:

$$\psi(x) = a_2 V_1(x;W) + \omega^{-1}(W) u_1(x;W) \int_0^\infty V_1(y;W)\eta(y)\mathrm{d}y + I_1(x;W),$$
$$I_1(x;W) = \omega^{-1}(W)\left[V_1(x;W)\int_0^x u_1(y;W)\eta(y)\mathrm{d}y \right.$$
$$\left. - u_1(x;W)\int_0^x V_1(y;W)\eta(y)\mathrm{d}y\right]. \quad (8.156)$$

Here, using the Cauchy–Schwarz inequality, one can see that $I_1(x) \sim O(x^{3/2})$ and $I_1'(x) \sim O(x^{1/2})$ as $x \to 0$.

Let us study the asymptotic behavior of functions $\psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$ as $x \to 0$ and as $x \to \infty$. Such functions can be considered square-integrable solutions of the equation

$$\check{H}\psi_* = \eta \in L^2(\mathbb{R}_+) \Longrightarrow (\check{H} - W)\psi_* = \tilde{\eta},\ \tilde{\eta} = \eta - W\psi_* \in L^2(\mathbb{R}_+). \quad (8.157)$$

Then, according to Theorem 7.1, we obtain $[\psi_*, \psi_*]|^\infty = 0$, $\forall \psi_* \in D^*_{\check{H}}(\mathbb{R}_+)$.

The aymptotics of the functions $\psi_*(x)$ and $\psi_*'(x)$ as $x \to 0$ are as follows: For $g_1 \geq 1/4$, we have

$$\psi_*(x) = O(x^{3/2}),\ \psi_*'(x) = O(x^{1/2}),\ x \to 0$$

(with logarithmic accuracy for $g_1 = 1/4$; see below).

For $g_1 < 1/4$, we use the general solution (8.156) and estimates $I_1(x) \sim O(x^{3/2})$ and $I_1'(x) \sim O(x^{1/2})$ as $x \to 0$. Then

$$\psi_*(x) = \psi_{*\mathrm{as}}(x) + \begin{cases} O(x^{3/2}),\ g_1 \neq 1/4, \\ O(x^{3/2}\sqrt{\ln x}),\ g_1 = 1/4, \end{cases}$$
$$\psi_*'(x) = \psi_{*\mathrm{as}}'(x) + \begin{cases} O(x^{1/2}),\ g_1 \neq 1/4, \\ O(x^{1/2}\sqrt{\ln x}),\ g_1 = 1/4, \end{cases}$$
$$\psi_{*\mathrm{as}}(x) = \begin{cases} 0,\ g_1 \geq 1/4, \\ a_1(cx)^{1/2+2\mu} + a_2(cx)^{1/2-2\mu},\ g_1 < 1/4. \end{cases} \quad (8.158)$$

As usual, starting with the s.a. differential operation $\check{H}$ with the potential (8.148), we construct the initial symmetric operator $\hat{H}$ defined on the domain $\mathcal{D}(\mathbb{R}_+)$. Its adjoint $\hat{H}^+$ is defined on the natural domain $D^*_{\check{H}}(\mathbb{R}_+)$.

8.10.1 Range 1

In this range, we have

$$g_1 \geq 1/4\ (\mu \geq 1/2).$$

Here $\Delta_{H^+}(\psi_*) = 0$. This means that the operator $\hat{H}^+$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x u_1(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_1}.$$

One can see that this functional belongs to the class A of simple guiding functionals considered in Sect. 5.4.1 with $U = u_1$ ($\tilde{U}$ is any solution of (8.149) with $\mathrm{Wr}\left(u_1, \tilde{U}\right) = 1$), and therefore the spectrum of $\hat{H}_1$ is simple.

The Green's function $G(x, y; W)$ of $\hat{H}_1$ and the derivative $\sigma'(E)$ of the spectral function have the form

$$G(x, y; W) = \omega^{-1}(W) \begin{cases} V_1(x; W)u_1(y; W),\ x > y, \\ u_1(x; W)V_1(y; W),\ x < y, \end{cases}$$

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \left[\frac{V_1(x_0; W)}{\omega(W)u_1(x_0; W)} \right]_{W=E+i0}.$$

For $m - 1 < 2\mu < m + 1$, $m \geq 1$, we have

$$V_1(x; W) = A_m(W)u_1(x; W) + \frac{\omega(W)}{4\mu c} V_{(m)}(x; W),$$

$$A_m(W) = \frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)} + a_m(W)\frac{\Gamma(\gamma_3)\Gamma(2\mu)\Gamma(\gamma_2)}{\Gamma(\alpha_1)\Gamma(\beta_1)},$$

$$V_{(m)}(x; W) = u_2\,(x; W) - a_m(W)\Gamma(\gamma_2)u_1\,(x; W)\,,$$

$$a_m(W) = \left.\frac{\Gamma(\alpha_2 + m)\Gamma(\beta_2 + m)}{m!\Gamma(\alpha_2)\Gamma(\beta_2)}\right|_{2\mu=m}.$$

As follows from (8.131), the function $V_{(m)}(x; W)$ exists for any W and for $m-1 < 2\mu < m + 1$. Note that $a_m(W)$ are polynomials in ν^2 and λ^2, i.e., in W, with real coefficients, so that $a_m(E)$ are real and $V_{(m)}(x; W)$ are real entire functions in W. It is a simple task to check that functions $A_m(W)$ exist for any W and for $m - 1 < 2\mu < m + 1$, and $A_m(E)$ are real. As a result, we obtain

$$\sigma'(E) = \pi^{-1} \operatorname{Im} \Omega^{-1}(W)\big|_{W=E+i0},\ \Omega(W) = \frac{\omega(W)}{A_m(W)},\ m - 1 < 2\mu < m + 1.$$

Since $\Omega^{-1}(W)$ is an analytic function of μ, its values at the points $\mu = m/2$ can be found as a limit $\mu \to m/2$. Then $\sigma'(E)$ for $\mu \neq m/2$ has the form

$$\sigma'(E) = -\frac{\Gamma(\gamma_2)}{4\pi c\mu\Gamma(\gamma_1)} \operatorname{Im} \Omega_1^{-1}(W)\big|_{W=E+i0},\ \Omega_1(W) = \frac{\Gamma(\alpha_2)\Gamma(\beta_2)}{\Gamma(\alpha_1)\Gamma(\beta_1)}.$$

For $E = 4c^2p^2 \geq 0$, $p \geq 0$, $\nu = -ip$, we obtain

$$\sigma'(E) = c^{-1} \sin h(2\pi p) \left(\frac{|\Gamma(\alpha_1)\Gamma(\beta_1)|}{2\pi\Gamma(\gamma_1)} \right)^2 > 0.$$

The function $\sigma'(E)$ is finite and positive for $E > 0$. It is finite and positive for $E = 0$ if $\lambda \neq 1/2 + n$, $n \in \mathbb{Z}_+$, and has an integrable singularity of the type $O(E^{-1/2})$ if $\lambda = 1/2 + n$, $n \in \mathbb{Z}_+$, so that all $E \in \mathbb{R}_+$ belong to the continuous spectrum of $\hat{H}_1$.

For $E = -4c^2\tau^2 < 0$, $\tau > 0$, $\nu = \tau$, the function $\Omega_1(E)$ reads

$$\Omega_1(E) = \frac{\Gamma(1/2 - \mu + \tau + \lambda)\Gamma(1/2 - \mu + \tau - \lambda)}{\Gamma(1/2 + \mu + \tau + \lambda)\Gamma(1/2 + \mu + \tau - \lambda)}.$$

If $g_2 \leq 0$, then $\Omega_1^{-1}(E)$ is finite real number for all τ (for all $E < 0$) and $\sigma'(E) = 0$, and the negative spectrum points are absent.

If $g_2 > 0$, then $\Omega_1^{-1}(E)$ can have nonzero imaginary part at the point where $\beta_2 = 1/2 + \mu + \tau - \lambda = -n$, $n \in \mathbb{Z}_+$, i.e., for energies

$$E_n = -4c^2 (\lambda - \mu - n - 1/2)^2 = -4c^2 \left(\sqrt{g_2} - \sqrt{g_1} - n - 1/2\right)^2.$$

The derivative of the spectral function has the form (there exist $n_{\max} + 1$ discrete levels)

$$\sigma'(E) = \sum_{n=0}^{n_{\max}} Q_n^2 \delta(E - E_n),\ Q_n = \sqrt{\frac{4c\tau_n \Gamma(\gamma_1 + n)\Gamma(\gamma_1 + 2\tau_n + n)}{n!\Gamma^2(\gamma_1)\Gamma(1 + 2\tau_n + n)}},$$

where

$$n_{\max} = \begin{cases} [K],\ K > [K], \\ [K] - 1,\ K = [K], \end{cases}$$

$$K = \lambda - \mu - 1/2 = \sqrt{g_2} - \sqrt{g_1} - 1/2.$$

Thus, there exists at least one discrete level ($n_{\max} \geq 0$) if $g_2 > (1/2 + \sqrt{g_1})^2$.

Finally, the simple spectrum of the operator $\hat{H}_1$ is given by

$$\operatorname{spec} \hat{H}_1 = \mathbb{R}_+ \cup \{E_n,\ n = 0, 1, \ldots, n_{\max}\}.$$

The (generalized) eigenfunctions

$$U(x; E) = \sqrt{\sigma'(E)} u_1(x; E),\ E \geq 0,$$

$$U_n(x) = Q_n u_1(x; E_n),\ E_n < 0,\ n = 0, 1, \ldots, n_{\max},$$

of the operator $\hat{H}_1$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

8.10.2 Range 2

In this range, we have

$$1/4 > g_1 > 0\ (1/2 > \mu > 0).$$

Using asymptotics (8.158), we obtain in the range under consideration: $\Delta_{H^+}(\psi_*) = -4\mu c(\overline{a_1}a_2 - \overline{a_2}a_1)$. This means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1 \cos\zeta = a_2 \sin\zeta$, $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$. Thus, in this range, there exists a family of s.a. operators $\hat{H}_{2,\zeta}$ parameterized by $\zeta \in \mathbb{S}(-\pi/2, \pi/2)$ with domains $D_{H_{2,\zeta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\begin{aligned} \psi(x) &= C\psi_{2,\zeta\mathrm{as}}(x) + O(x^{3/2}), \\ \psi'(x) &= C\psi'_{2,\zeta\mathrm{as}}(x) + O(x^{1/2}), \\ \psi_{2,\zeta\mathrm{as}}(x) &= (cx)^{1/2+2\mu}\sin\zeta + (cx)^{1/2-2\mu}\cos\zeta. \end{aligned} \tag{8.159}$$

Therefore,

$$D_{H_{2,\zeta}} = \left\{\psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy (8.159)}\right\}.$$

Imposing the boundary conditions (8.159) on the functions (8.156) and using the asymptotics (8.155), we obtain Green's functions of the Hamiltonians $\hat{H}_{2,\zeta}$,

$$\begin{aligned} G(x, y; W) &= \Omega^{-1}(W)U_{2,\zeta}(x; W)U_{2,\zeta}(y; W) \\ &\quad - \frac{1}{4\mu c}\begin{cases} \tilde{U}_{2,\zeta}(x; W)U_{2,\zeta}(y; W),\ x > y, \\ U_{2,\zeta}(x; W)\tilde{U}_{2,\zeta}(x; W),\ x < y. \end{cases} \end{aligned} \tag{8.160}$$

Here

$$\begin{aligned} U_{2,\zeta}(x; W) &= u_1(x; W)\sin\zeta + u_2(x; W)\cos\zeta, \\ \tilde{U}_{2,\zeta}(x; W) &= u_1(x; W)\cos\zeta - u_2(x; W)\sin\zeta, \\ \Omega(W) &= -\frac{4\mu c[f(W)\cos\zeta + \sin\zeta]}{f(W)\sin\zeta - \cos\zeta},\ f(W) = \frac{\Gamma(\gamma_2)\Gamma(\alpha_1)\Gamma(\beta_1)}{\Gamma(\gamma_1)\Gamma(\alpha_2)\Gamma(\beta_2)}, \\ V_1(x; W) &= \tilde{\omega}_{2,\nu}(W)U_{2,\zeta}(x; W) - \omega_{2,\zeta}(W)\tilde{U}_{2,\zeta}(x; W), \\ \omega_{2,\zeta}(W) &= q_1(W)\cos\zeta + q_2(W)\sin\zeta, \\ \tilde{\omega}_{2,\zeta}(W) &= q_1(W)\sin\zeta - q_2(W)\cos\zeta, \\ q_1(W) &= -\frac{\Gamma(\gamma_3)\Gamma(-2\mu)}{\Gamma(\alpha_2)\Gamma(\beta_2)},\ q_2(W) = \frac{\Gamma(\gamma_3)\Gamma(2\mu)}{\Gamma(\alpha_1)\Gamma(\beta_1)} = \frac{\omega(W)}{4\mu c}. \end{aligned} \tag{8.161}$$

Note that $U_{2,\zeta}$ and $\tilde{U}_{2,\zeta}$ are solutions of (8.149) real entire in W, $U_{2,\zeta}$ satisfies the boundary condition (8.159), and the second summand on the right-hand side of (8.160) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi; W) = \int_0^\infty \mathrm{d}x\, U_{2,\zeta}(x; W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{2,\zeta}}.$$

One can see that this functional belongs to the class B of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{2,\zeta}$ ($\tilde{U} = \tilde{U}_{2,\zeta}$), and therefore the spectra of $\hat{H}_{2,\zeta}$ are simple.

The derivative of the spectral function reads $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

We first consider the extension with $\zeta = \pi/2$. In this case, $U_{2,\pi/2} = u_1$ and

$$\sigma'(E) = -(4\pi\mu c)^{-1}\,\mathrm{Im}\, f(E + i0).$$

We can see that the spectrum and inversion formulas coincide with those in the first region for $0 < g_1 < 1/4$ $(0 < \mu < 1/2)$. In particular, the energy levels $E_n|_{\zeta=\pi/2} \equiv \mathcal{E}_n$,

$$\mathcal{E}_n = -4c^2(\sqrt{g_2} - \sqrt{g_1} - 1/2 - n)^2,\ n = 0, 1, \ldots, n_{\max},$$
$$n_{\max} = \begin{cases} \left[K_{\pi/2}\right],\ K_{\pi/2} > \left[K_{\pi/2}\right], \\ \left[K_{\pi/2}\right] - 1,\ K_{\pi/2} = \left[K_{\pi/2}\right], \end{cases} \qquad K_{\pi/2} = \sqrt{g_2} - \sqrt{g_1} - 1/2.$$

and the levels $\mathcal{E}_n$ exist only for $g_2 > 0$, $\sqrt{g_2} - \sqrt{g_1} > 1/2$.

We obtain the same results for the case $\zeta = -\pi/2$.

Let us consider the extension with $\zeta = 0$. In this case, $U_{2,\pi/2} = u_2$ and $\sigma'(E) = (4\pi\mu c)^{-1}\,\mathrm{Im}\, f^{-1}(E + i0)$. Here, the spectrum and inversion formulas coincide with those in the first region if we replace μ by $-\mu$. In particular, the energy levels $E_n|_{\zeta=0} \equiv E_n\,(0)$ are

$$E_n\,(0) = -4c^2(\sqrt{g_2} + \sqrt{g_1} - 1/2 - n)^2,\ n = 0, 1, \ldots, n_{\max},$$
$$n_{\max} = \begin{cases} [K_0],\ K_0 > [K_0], \\ [K_0] - 1,\ K_0 = [K_0], \end{cases} \qquad K_0 = \sqrt{g_2} + \sqrt{g_1} - 1/2,$$

and the levels $E_n\,(0)$ exist only for $g_2 > 0$, $\sqrt{g_2} + \sqrt{g_1} > 1/2$.

Let us consider extensions with $|\zeta| < \pi/2$. For such extensions, we have

$$\sigma'(E) = \mathrm{Im}\left[4\pi\mu c\cos^2\zeta f_\zeta(E + i0)\right]^{-1} = \sum_{n\in\Lambda} Q_n^2\delta(E - E_n\,(\zeta)),$$
$$Q_n = \sqrt{[4\mu c\cos^2\zeta f'(E_n\,(\zeta))]^{-1}},\ f'(E_n\,(\zeta)) < 0,$$

where $\Lambda = \{0, \ldots, n_{\max}\}$, see below, and

$$f_\zeta(W) = f(W) + \tan\zeta,\ f(E_n\,(\zeta)) = -\tan\zeta,$$
$$\partial_\zeta E_n\,(\zeta) = -\left[f'(E_n\,(\zeta))\cos^2\zeta\right]^{-1} > 0.$$

The function $f(W)$ is given by (8.161). One can see that $f(E)$ is real; $f(E) \to \infty$ as $E \to -\infty$; if there exists a level $\mathcal{E}_n$, $n \in \mathbb{Z}_+$, then the level $E_n\,(0)$ exists as well, and $E_n\,(0) < \mathcal{E}_n$; if there exists a level $E_{n+1}\,(0)$, $n \in \mathbb{Z}_+$, then the level $\mathcal{E}_n$ exists as well, and $\mathcal{E}_n < E_{n+1}\,(0)$.

Then we obtain the following:

(1) Let $g_2 \leq 0$ or $g_2 > 0$, $\sqrt{g_2} < 1/2 + \sqrt{g_1}$. Here the function $f(E)$ is monotonically decreasing and smooth for $E \in (\mathcal{E}_{-1}, 0)$ (we set $\mathcal{E}_{-1} = -\infty$). For $\zeta \in [\zeta_1, \pi/2)$, $\zeta_1 = -\arctan f(-0)$, there are no negative discrete energy levels ($n_{\max} = -1$); for any $\zeta \in (-\pi/2, \zeta_1)$, there is one discrete level $E_0(\zeta)$ ($n_{\max} = 0$), which monotonically increases from $\mathcal{E}_{-1} + 0$ to -0 as ζ goes from $-\pi/2$ to $\zeta_1 - 0$.
(2) Let $\sqrt{g_2} - \sqrt{g_1} = 1/2 + k$, $k \in \mathbb{N}$. Here, we have $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \dots, k-1$, $f(-0) = -\infty$. For any fixed $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n = 0, \dots, k$ (here we set $\mathcal{E}_k = 0$), there exists one discrete level $E_n(\zeta)$ ($n_{\max} = k$), which monotonically increases from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ as ζ goes from $\pi/2 - 0$ to $-\pi/2 + 0$.
(3) Let $1/2 + k < \mu + \lambda < 1/2 + k + 1$, $k \in \mathbb{Z}_+$. Here, we have

$$f(\mathcal{E}_n \pm 0) = \pm\infty,\ n = 0, \dots, k,\ |f(-0)| < \infty.$$

For any $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n = 0, \dots, k$, there exists one discrete level $E_n(\zeta)$, which monotonically increases from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ as ζ goes from $-\pi/2 + 0$ to $\pi/2 - 0$. For any $\zeta \in [\zeta_1, \pi/2)$, there are no other discrete levels ($n_{\max} = k$). For any $\zeta \in (-\pi/2, \zeta_1)$ there exists one discrete level $E_{k+1}(\zeta) \in (\mathcal{E}_k, 0)$ ($n_{\max} = k + 1$), which monotonically increases from $\mathcal{E}_k + 0$ to -0 as ζ goes from $-\pi/2 + 0$ to $\zeta_1 - 0$.

8.10.3 Range 3

In this range, we have

$$g_1 = \mu = 0.$$

Here, we use the following solutions of (8.149):

$$\begin{aligned}
u_1(x; W) &= z^{1/4}(1-z)^\nu F(\alpha, \beta; 1; z) = u_1(x; W)|_{\nu \to -\nu}, \\
u_3(x; W) &= \frac{\partial}{\partial \mu}\left[u_1(x; W)|_{\mu \neq 0}\right]_{\mu = 0;\ \nu, \lambda \text{ are fixed}} \\
&= z^{1/4}(1-z)^\nu \ln z F(\alpha, \beta; 1; z) \\
&\quad + z^{1/4}(1-z)^\nu \frac{\partial}{\partial \mu} F(\alpha_1, \beta_1; \gamma_1; z)|_{\mu \neq 0}\Big|_{\mu = 0;\ \nu, \lambda \text{ are fixed}} = u_3(x; W)|_{\nu \to -\nu},
\end{aligned}$$

$$V_1(x; W) = z^{1/4}(1-z)^\nu F(\alpha, \beta; \gamma; 1 - z),\ \alpha = \alpha_+,\ \alpha_\pm = 1/2 \pm \nu + \lambda,$$
$$\beta = \beta_+,\ \beta_\pm = 1/2 \pm \nu - \lambda,\ \gamma = \gamma_+,\ \gamma_\pm = 1 \pm 2\nu.$$

The solutions $u_1\,(x;W)$ and $u_3\,(x;W)$ are real entire in W. The following relations hold:

$$V_1\,(x;W) = -\frac{\partial}{\partial\mu}\left[\frac{\Gamma(\gamma_3)\Gamma(\gamma_2)}{\Gamma(\alpha_2)\Gamma(\beta_2)}u_1\,(x;W)\bigg|_{\mu\neq 0}\right]_{\mu=0;\ \nu,\lambda\ \text{are fixed}}$$

$$= j\,(W)\,\Gamma(\gamma)u_1\,(x;W) - \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}u_3\,(x;W)\,,$$

$$j\,(W) = \frac{\partial}{\partial\mu}\frac{\Gamma(\gamma_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)}\bigg|_{\mu=0;\ \nu,\lambda\ \text{are fixed}} = -\frac{2\mathbf{C}+\psi(\alpha)+\psi(\beta)}{\Gamma(\alpha)\Gamma(\beta)}.$$

Below, we list some asymptotics of the introduced functions as $x\to 0$ and $x\to\infty$; see [1, 20, 81].

As $x\to 0$, $z=(cx)^2\tilde{O}(x^2)\to 0$, we have

$$u_1(x;W) = z^{1/4}\tilde{O}(z) = (cx)^{1/2}\tilde{O}(x^2),$$
$$u_3(x;W) = z^{1/4}\,(\ln z)\,\tilde{O}(z\ln z) = 2(cx)^{1/2}(\ln cx)\tilde{O}(x^2\ln x),$$
$$V_1(x;W) = (cx)^{1/2}\left[j\,(W)\,\Gamma(\gamma) - 2\frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\ln(cx)\right]\tilde{O}(x^2\ln x). \qquad (8.162)$$

As $x\to\infty$, $1-z = 4\mathrm{e}^{-2cx}\tilde{O}(\mathrm{e}^{-2cx})\to 0$, $z\to 1$, $\operatorname{Im} W>0$, we have

$$V_1(x;W) = 4^{\nu}\mathrm{e}^{-2\nu cx}\tilde{O}\left(\mathrm{e}^{-2cx}\right),$$
$$u_1(x;W) = \frac{\Gamma(2\nu)}{4^{\nu}\Gamma(\alpha)\Gamma(\beta)}\mathrm{e}^{2\nu cx}\tilde{O}(\mathrm{e}^{-2cx}).$$

We stress that $V_1\,(x;W)$ is square-integrable at the origin.

Since

$$\operatorname{Wr}(u_1,u_2) = 2c,\ \operatorname{Wr}(u_1,V_1) = -\frac{2c\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} = -\omega(W),$$

the solutions u_1 and V_1 form a fundamental set $\operatorname{Im} W\neq 0$ and $W=0$.

Let us study asymptotics of functions $\psi_*\in D^*_{\check{H}}(\mathbb{R}_+)$ as $x\to 0$ and as $x\to\infty$. Such functions can be considered square-integrable solutions of (8.157) with the following asymptotics as $x\to 0$:

$$\psi_*(x) = \psi_{\text{as}}(x) + O(x^{3/2}\ln x),\ \psi_*'(x) = \psi_{\text{as}}'(x) + O(x^{1/2}\ln x),$$
$$\psi_{\text{as}}(x) = a_1(cx)^{1/2} + 2a_2(cx)^{1/2}\ln(cx).$$

As in the previous ranges, here we have $[\psi_*,\psi_*]|^{\infty} = 0$ and $\Delta_{H^+}(\psi_*) = 2c(\overline{a_1}a_2 - \overline{a_2}a_1)$, which means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1\cos\zeta = a_2\sin\zeta$, $\zeta\in\mathbb{S}(-\pi/2,\pi/2)$. Thus, in the range under consideration, there exists a family of s.a. operators $\hat{H}_{3,\zeta}$ parameterized by ζ with domains $D_{H_{3,\zeta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$,

$$\begin{aligned}\psi(x) &= C\psi_{3,\zeta\mathrm{as}}(x) + O(x^{3/2}\ln x),\\ \psi'(x) &= C\psi'_{3,\zeta\mathrm{as}}(x) + O(x^{1/2}\ln x),\\ \psi_{3,\zeta\mathrm{as}}(x) &= (cx)^{1/2}\sin\zeta + 2(cx)^{1/2}\ln(cx)\cos\zeta.\end{aligned} \tag{8.163}$$

Therefore,

$$D_{H_{3,\zeta}} = \{\psi \in D^*_{\check{H}}(\mathbb{R}_+),\ \psi \text{ satisfy (8.163)}\}.$$

Imposing the boundary conditions (8.163) on the functions (8.156) and using the asymptotics (8.162), we obtain the Green's function of $\hat{H}_{3,\zeta}$,

$$\begin{aligned}G(x,y;W) &= \Omega^{-1}(W)U_{3,\zeta}(x;W)U_{3,\zeta}(y;W)\\ &\quad + \frac{1}{2c}\begin{cases}\tilde{U}_{3,\zeta}(x;W)U_{3,\zeta}(y;W),\ x>y,\\ U_{3,\zeta}(x;W)\tilde{U}_{3,\zeta}(y;W),\ x<y,\end{cases}\end{aligned} \tag{8.164}$$

where

$$\begin{aligned}&\Omega(W) = \frac{2c\omega_{3,\zeta}(W)}{\tilde{\omega}_{3,\zeta}(W)},\ \omega_{3,\zeta}(W) = f(W)\cos\zeta - \sin\zeta,\\ &\tilde{\omega}_{3,\zeta}(W) = f(W)\sin\zeta + \cos\zeta,\ f(W) = 2\mathbf{C} + \psi(\alpha) + \psi(\beta),\\ &U_{3,\zeta}(x;W) = u_1(x;W)\sin\zeta + u_3(x;W)\cos\zeta,\\ &\tilde{U}_{3,\zeta}(x;W) = u_1(y;W)\cos\zeta - u_3(x;W)\sin\zeta,\\ &2c\omega^{-1}(W)V_1(x;W) = -\tilde{\omega}_{3,\zeta}(W)U_{3,\zeta}(x;W) - \omega_{3,\zeta}(W)\tilde{U}_{3,\zeta}(x;W).\end{aligned} \tag{8.165}$$

We note that $U_{3,\zeta}$ and $\tilde{U}_{3,\zeta}$ are solutions of (8.149) real entire in W, $U_{3,\zeta}$ satisfies the boundary condition (8.163), and the second summand on the right-hand side of (8.164) is real for real $W = E$.

Consider the guiding functional

$$\Phi(\xi;W) = \int_0^\infty \mathrm{d}x U_{3,\zeta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+)\cap D_{H_{3,\zeta}}.$$

One can see that this functional belongs to the class C of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{3,\zeta}$ ($\tilde{U} = \tilde{U}_{3,\zeta}$), and therefore the spectra of $\hat{H}_{3,\zeta}$ are simple.

Using the Green's function, we obtain the derivative of the spectral function, $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

Let us consider the extension with $\zeta = \pi/2$. In this case, we have $U_{3,\pi/2}(x;W) = u_1(x;W)$, and

$$\sigma'(E) = -\frac{1}{2\pi c}\,\mathrm{Im}\,[\psi(\alpha)+\psi(\beta)]|_{W=E+i0}\,.$$

For $E = 4c^2p^2 \geq 0$, $p \geq 0$, $\nu = -ip$, we have

$$\sigma'(E) = \frac{\sin h(2\pi p).}{2c\,[\cos h(2\pi p) + \cos(2\pi\lambda)]}. \tag{8.166}$$

The function (8.166) is finite and positive for $E > 0$; if $\lambda \neq 1/2 + n$, $n \in \mathbb{Z}_+$, $\sigma'(0) = 0$; if $\lambda = 1/2 + n$, $n \in \mathbb{Z}_+$, the function $\sigma'(E)$ has an integrable singularity of type $O(E^{-1/2})$. Therefore, all $E \in \mathbb{R}_+$ belong to the continuous spectrum of $\hat{H}_{3,\pi/2}$.

For $E = -4c^2\tau^2 < 0$, $\tau > 0$, $\nu = \tau$, the function $\psi(\alpha) + \psi(\beta)$ is real, so that $\sigma'(E)$ can be different from zero only at the points $\mathcal{E}_n$ where $\psi(\beta)$ is infinite. This is possible only for $g_2 > 1/4$, where we have

$$\sigma'(E) = \sum_{n=0}^{n_{\max}} Q_n^2\delta(E-\mathcal{E}_n),\ Q_n = (3|\mathcal{E}_n|)^{1/4}\,,$$

$$\mathcal{E}_n = -4c^2\left(\sqrt{g_2} - 1/2 - n\right)^2,$$

$$n_{\max} = \begin{cases} [K]\,,\ K > [K]\,, \\ [K]-1,\ K = [K]\,, \end{cases} \qquad K = \sqrt{g_2} - 1/2.$$

Finally, the simple spectrum of $\hat{H}_{3,\pi/2}$ is given by

$$\mathrm{spec}\ \hat{H}_{3,\pi/2} = \mathbb{R}_+ \cup \{\mathcal{E}_n,\ n = 0, 1, \ldots, n_{\max}\}.$$

The set of (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}U_{3,\pm\pi/2}(x; E),\ E \geq 0,$$

$$U_n(x) = Q_n U_{3,\pi/2}(x; \mathcal{E}_n),\ n = 0, 1, \ldots, n_{\max},$$

of $\hat{H}_{3,\pi/2}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

The same results hold for $\zeta = -\pi/2$.

Let us note that the solution of the spectral problem in the case under consideration can be obtained from the corresponding solution of the first range $g_1 \geq 1/4$ in the limit $\mu \to 0$.

Now we consider extensions with $|\zeta| < \pi/2$. For such extensions, we have

$$\sigma'(E) = \left(2\pi c\cos^2\zeta\right)^{-1}\mathrm{Im}\,f_\zeta^{-1}(E+i0),\ f_\zeta(W) = f(W) - \tan\zeta,$$

where $f(W)$ is given by (8.165).

For $E = 4c^2p^2 \geq 0$, $p \geq 0$, $\nu = -ip$, we obtain

$$\sigma'(E) = \frac{B(E)}{2\pi c[(A(E)-\tilde{\zeta})^2 + B^2(E)]},$$

where $[\psi(\alpha) + \psi(\beta)]_{W=E} = A(E) - iB(E)$, and $\tilde{\zeta} = \tan\zeta - 2\mathbf{C}$. The function $B(E)$ can be explicitly calculated:

$$B(E) = \frac{\pi \sin h(2\pi p).}{\cos h(2\pi p) + \cos(2\pi\lambda)} \geq 0.$$

Thus, $\sigma'(E)$ is finite and positive for $E > 0$. It can have an integrable singularity of type $O(E^{-1/2})$ as $E \to 0$, so that all $E \in \mathbb{R}_+$ belong to the continuous spectrum of $\hat{H}_{3,\zeta}$.

For $E = -4c^2\tau^2 < 0$, $\tau > 0$, $\nu = \tau$, the function $f_\zeta(E)$,

$$f_\zeta(E) = f(E) - \tan\zeta,\ f(E) = \psi(1/2 + \tau + \lambda) + \psi(1/2 + \tau - \lambda) + 2\mathbf{C},$$
$$f(E) = \ln|E| + O(1) \to \infty \text{ as } E \to -\infty,$$

is real, so that only the points $E_n(\zeta)$ that satisfy the equation $f_\zeta(E_n(\zeta)) = 0$ can contribute to $\sigma'(E)$. That is why

$$\sigma'(E) = \sum_{n=\Lambda} Q_n^2 \delta(E - E_n(\zeta)),\ Q_n = \left[-2c\cos^2\zeta f_\zeta'(E_n(\zeta))\right]^{-1/2},$$

where

$$f_\zeta'(E_n(\zeta)) < 0,\ f(E_n(\zeta)) = \tan\zeta,$$
$$\partial_\zeta E_n(\zeta) = \left[f'(E_n(\zeta))\cos^2\zeta\right]^{-1} < 0.$$

Finally, the simple spectrum of the s.a. Hamiltonian $\hat{H}_{3,\zeta}$ is given by

$$\operatorname{spec} \hat{H}_{3,\zeta} = \mathbb{R}_+ \cup \{E_n(\zeta) < 0,\ n \in \Lambda\},$$

where $\Lambda = \{0, 1, \ldots, n_{\max}\}$.

The set of (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)} U_{3,\zeta}(x; E),\ E \geq 0,$$
$$U_n(x) = Q_n U_{3,\zeta}(x; E_n(\zeta)),\ n \in \Lambda,$$

of $\hat{H}_{3,\zeta}$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

Some remarks on the spectrum structure can be made:

(1) Let $g_2 \leq 1/4$. Then $f(E)$ is smooth on $(\mathcal{E}_{-1}, 0)$ (we set $\mathcal{E}_{-1} = -\infty$). In this region, there are no discrete negative levels ($n_{\max} = -1$) for extensions with $\zeta \in (-\pi/2, \zeta_1]$, $\zeta_1 = \arctan f(-0)$. For any fixed $\zeta \in (\zeta_1, \pi/2)$, there is one discrete level $E_{10}(\zeta)$ ($n_{\max} = 0$), which monotonically increases from $\mathcal{E}_{-1}$ to -0 as ζ goes from $\pi/2 - 0$ to $\zeta_1 + 0$.

(2) Let $\lambda = 1/2 + k$, $k \in \mathbb{N}$. Then $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \ldots, k-1$, $f(-0) = -\infty$. For such a region of parameters, for any fixed $\zeta \in (-\pi/2, \pi/2)$, in each interval

$(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n = 0, \ldots, k$ (in this item only, we set $\mathcal{E}_k = 0$), there exists one discrete level $E_n(\zeta)$ ($n_{\max} = k$), which monotonically increases from $\mathcal{E}_{n-1} + 0$ to $\mathcal{E}_n - 0$ as ζ goes from $\pi/2 - 0$ to $-\pi/2 + 0$.

(3) Let $1/2+k < \mu+\lambda < 1/2+k+1$, $k \in \mathbb{Z}_+$, then $f(\mathcal{E}_n \pm 0) = \pm\infty$, $n = 0, \ldots, k$, $|f_3(-0)| < \infty$. For such region of parameters, for any fixed $\zeta \in (-\pi/2, \pi/2)$, in each interval $(\mathcal{E}_{n-1}, \mathcal{E}_n)$, $n = 0, \ldots, k$, there exists one discrete level $E_n(\zeta)$, which monotonically increases from $\mathcal{E}_{n-1}+0$ to $\mathcal{E}_n-0$ as ζ goes from $\pi/2-0$ to $-\pi/2+0$. For any $\zeta \in (-\pi/2, \zeta_1]$, there are no other discrete eigenvalues ($n_{\max} = k$). For any fixed $\zeta \in (\zeta_1, \pi/2)$, there is one ($n_{\max} = k + 1$) discrete level $E_{k+1}(\zeta) \in (\mathcal{E}_k, 0)$, which monotonically increases from $\mathcal{E}_k + 0$ to -0 as ζ goes from $\pi/2 - 0$ to $\zeta_1 + 0$.

8.10.4 Range 4

In this range, we have

$$g_1 < 0 \; (\mu = i\varkappa, \; \varkappa > 0).$$

Using the asymptotics (8.158) and the fact that $[\psi_*, \psi_*]|^\infty = 0$, we obtain $\Delta_{H^+}(\psi_*) = 4i\varkappa c(\overline{a_2}a_2 - \overline{a_1}a_1)$. This means that the deficiency indices of $\hat{H}$ are $m_\pm = 1$. The condition $\Delta_{H^+}(\psi_*) = 0$ implies $a_1 = e^{2i\theta}a_2$, $\theta \in \mathbb{S}(0, \pi)$. Thus, in the range under consideration, there exists a family of s.a. operators $\hat{H}_{4,\theta}$ parameterized by θ with domains $D_{H_{4,\theta}}$ that consist of functions from $D^*_{\check{H}}(\mathbb{R}_+)$ with the following asymptotic behavior as $x \to 0$:

$$\begin{aligned} \psi(x) &= C\psi_{4,\theta\text{as}}(x) + O(x^{3/2}), \\ \psi'(x) &= C\psi'_{4,\theta\text{as}}(x) + O(x^{1/2}), \\ \psi_{4,\theta\text{as}}(x) &= e^{i\theta}(cx)^{1/2+2i\varkappa} + e^{-i\theta}(cx)^{1/2-2i\varkappa}. \end{aligned} \tag{8.167}$$

Therefore,

$$D_{H_{4,\theta}} = \{\psi \in D^*_{\check{H}}(\mathbb{R}_+), \; \psi \text{ satisfy } (8.167)\}.$$

Imposing the boundary conditions (8.167) on the functions (8.156) and using the asymptotics (8.155), we obtain the Green's functions of the Hamiltonians $\hat{H}_{4,\theta}$,

$$\begin{aligned} G_{4,\theta}(x, y; W) &= \Omega^{-1}(W)U_{4,\theta}(x; W)U_{4,\theta}(y; W) \\ &\quad - \frac{1}{8\varkappa c}\begin{cases} \tilde{U}_{4,\theta}(x; W)U_{4,\theta}(y; W), & x > y, \\ U_{4,\theta}(x; W)\tilde{U}_{4,\theta}(y; W), & x < y. \end{cases} \end{aligned} \tag{8.168}$$

Here

$$\Omega = i\frac{8\varkappa c\omega_{4,\theta}(W)}{\tilde{\omega}_{4,\theta}(W)}, \; \omega_{4,\theta}(W) = e^{i\theta}a(W) + e^{-i\theta}b(W),$$

$$\tilde{\omega}_{4,\theta}(W) = e^{i\theta}a(W) - e^{-i\theta}b(W),$$

$$
\begin{aligned}
a(W) &= \frac{\Gamma(\gamma_3)\Gamma(\gamma_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)},\ b(W) = \frac{\Gamma(\gamma_3)\Gamma(\gamma_2)}{\Gamma(\alpha_2)\Gamma(\beta_2)},\\
U_{4,\theta}(x;W) &= \mathrm{e}^{i\theta}u_1(x;W) + \mathrm{e}^{-i\theta}u_2(x;W),\\
\tilde{U}_{4,\theta}(x;W) &= i[\mathrm{e}^{-i\theta}u_2(x;W) - \mathrm{e}^{i\theta}u_1(x;W)],\\
4\mu V_1(x;W) &= \tilde{\omega}_{4,\theta}(W)U_{4,\theta}(x;W) - i\omega_{4,\theta}(W)\tilde{U}_{4,\theta}(x;W).
\end{aligned}
$$

Note that $U_{4,\theta}$ and $\tilde{U}_{4,\theta}$ are solutions of (8.149) real entire in W, $U_{4,\theta}$ satisfies boundary conditions (8.167), and the second summand on the right-hand side of (8.168) is real for real $W = E$.

Consider the guiding functional

$$
\Phi(\xi;W) = \int_0^\infty \mathrm{d}x U_{4,\theta}(x;W)\xi(x),\ \xi \in \mathcal{D}_r(\mathbb{R}_+) \cap D_{H_{4,\theta}}.
$$

One can see that this functional belongs to the class D of simple guiding functionals considered in Sect. 5.4.1 with $U = U_{4,\theta}$ ($\tilde{U} = \tilde{U}_{4,\theta}$), and therefore the spectra of $\hat{H}_{4,\theta}$ are simple.

The derivative of the spectral function reads $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\Omega^{-1}(E + i0)$.

For $E = 4c^2p^2 \geq 0$, $p \geq 0$, $\nu = -ip$, we have $\mathrm{Im}\,\Omega^{-1}(E + i0) = \mathrm{Im}\,\Omega^{-1}(E)$, and

$$
\Omega^{-1}(E) = \frac{i\pi\left[\mathrm{e}^{i\theta}\Gamma(\gamma_1)\Gamma(\alpha_2)\Gamma(\beta_2) - \mathrm{e}^{-i\theta}\Gamma(\gamma_2)\Gamma(\alpha_1)\Gamma(\beta_1)\right]}{8\pi\varkappa c\left[\mathrm{e}^{i\theta}\Gamma(\gamma_1)\Gamma(\alpha_2)\Gamma(\beta_2) + \mathrm{e}^{-i\theta}\Gamma(\gamma_2)\Gamma(\alpha_1)\Gamma(\beta_1)\right]}.
$$

One can verify that $\sigma'(E)$ is finite and positive for $E > 0$. It can have an integrable singularity of the type $O(E^{-1/2})$ as $E \to 0$, so that all $E \in \mathbb{R}_+$ belong to the continuous spectrum of $\hat{H}_{4,\theta}$.

For $E = -4c^2\tau^2 < 0$, $\tau > 0$, $\nu = \tau$, we have $\Omega(E) = 8\varkappa c \cot\Theta(E)$, where $\Theta(E) = f(E) + \theta$,

$$
\begin{aligned}
f(E) = \frac{1}{2i}&\left[\ln\Gamma(1+2i\varkappa) - \ln\Gamma(1-2i\varkappa)\right]\\
&+ \frac{1}{2i}\left[\ln\Gamma(1/2 - i\varkappa + \tau + \lambda) - \ln\Gamma(1/2 + i\varkappa + \tau + \lambda)\right]\\
&+ \frac{1}{2i}\left[\ln\Gamma(1/2 - i\varkappa + \tau - \lambda) - \ln\Gamma(1/2 + i\varkappa + \tau - \lambda)\right].
\end{aligned}
$$

Thus, only the points $E_n(\theta)$ that satisfy the equation

$$
\Theta(E_n(\theta)) = \frac{\pi}{2} - \pi n,\ n \in \mathbb{Z}, \tag{8.169}
$$

can contribute to $\sigma'(E)$. Thus, we obtain

$$
\sigma'(E) = \sum_n Q_n^2\delta\left(E - E_n(\theta)\right),\ Q_n = \left[8\varkappa c\Theta'(E_n(\theta))\right]^{-1/2},\ \Theta'(E_n(\theta)) > 0.
$$

Finally, the simple spectra of $\hat{H}_{4,\theta}$ are given by

$$\operatorname{spec} \hat{H}_{4,\theta} = \mathbb{R}_+ \cup \{E_n(\theta),\ n \in \mathbb{Z}\}.$$

The sets of (generalized) eigenfunctions

$$U_E(x) = \sqrt{\sigma'(E)}U_{4,\theta}(x;E),\ E \geq 0,$$

$$U_n(x) = Q_n U_{4,\theta}(x;E_n(\theta)),\ n \in \mathbb{Z},$$

of $\hat{H}_{4,\theta}$ form complete orthonormalized systems in $L^2(\mathbb{R}_+)$.

Some remarks on the spectrum structure can be made. Let us rewrite the spectrum equation (8.169) as follows:

$$f(E_n(\theta)) = \pi/2 + \pi n_0 - \pi(n + \theta/\pi),\ n \in \mathbb{Z}, \tag{8.170}$$

where

$$n_0 = [1/2 + f(0)/\pi],\ f(0) = \pi/2 + \pi n_0 - \theta_0,\ 0 < \theta_0 \leq \pi.$$

We note that

$$f(E) = -\varkappa \ln(|E|/4c^2) + O(1),\ E \to -\infty;$$

$$f'(E_n(\theta)) > 0,\ \partial_\theta E_n(\theta) = -1/f'(E_n(\theta)) < 0.$$

Then, one can see that (8.170) has no solutions for $n \leq -1$, so that $n \in \mathbb{Z}_+$; for $n = 0$ and $\theta \in [0, \theta_0]$, (8.170) has no solutions; for $n = 0$ and $\theta \in (\theta_0, \pi)$, (8.170) has only one solution $E_0(\theta) \in (E_0(\pi) = E_1(0), 0)$, which monotonically increases from $E_0(\pi) + 0$ to -0 as θ goes from $\pi - 0$ to $\theta_0 + 0$; in each interval $(E_n(\pi) = E_{n+1}(0), E_n(0)]$, $n \in \mathbb{N}$, there exists only one discrete level $E_n(\theta)$ for a given $\theta \in [0, \pi)$, which monotonically increases from $E_n(\pi) + 0$ to $E_n(0)$ as θ goes from $\pi - 0$ to 0. In particular, $E_{n+1}(0) < E_n(0)$, $\forall n \in \mathbb{Z}_+$.

We note also that in the range under consideration, the spectrum of $\hat{H}_{4,\theta}$ is unbounded from below and asymptotically coincides with the spectrum of the Calogero Hamiltonian with $\alpha = 4g_1 - 1/4 = (V_1 + V_2)/4c^2$ and $k_0 = c$ for high negative energies.

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In this case,

$$V(x) = 4c^2 \frac{1/16 - g_1 + g_2 \sin h(cx)}{\cos h^2(cx)},\ x \in \mathbb{R}, \tag{8.171}$$

and the corresponding Schrödinger equation is

$$\psi'' - 4c^2 \frac{1/16 - g_1 + g_2 \sin h(cx)}{\cos h^2(cx)} \psi + W\psi = 0. \tag{8.172}$$

It is sufficient to consider only the case $c > 0$ and $g_2 > 0$ without loss of generality. Let us introduce a new variable z,

$$z = \left(\frac{\upsilon + i}{\upsilon - i} \right)^2, \ \upsilon = \mathrm{e}^{cx},$$

and parameters μ, λ, and ν:

$$\begin{aligned} \mu &= \sqrt{g_1 + i g_2}, \ \lambda = \sqrt{g_1 - i g_2}, \ \nu = \sqrt{-Wc^{-2}} \\ &= \sqrt{|W|c^{-2}}[\sin(\varphi/2) - i \cos(\varphi/2)], \ W = |W|\mathrm{e}^{i\varphi}, \ 0 \le \varphi \le \pi. \end{aligned}$$

We note that the path $-\infty \Longrightarrow \infty$ of the variable x along the real axis corresponds to the path $1 - i0 \Longrightarrow 1 + i0$ of the variable z in the complex plane along (clockwise) a circle $|z| = 1$.

In addition, we introduce new functions $\phi_{\xi_\mu}(z)$,

$$\psi(x) = (-z)^{1/4 + \xi_\mu \mu}(1 - z)^\nu \phi_{\xi_\mu}(z), \ \xi_\mu = \pm \, . \tag{8.173}$$

They satisfy the following equations:

$$\begin{aligned} &z(1 - z)d_z^2 \phi_{\xi_\mu}(z) + [\gamma_{\xi_\mu} - (1 + \alpha_{\xi_\mu} + \beta_{\xi_\mu})z]d_z \phi_{\xi_\mu}(z) \\ &\quad - \alpha_{\xi_\mu} \beta_{\xi_\mu} \phi_{\xi_\mu}(z) = 0, \ \alpha_{\xi_\mu} = 1/2 + \xi_\mu \mu + \nu + \lambda, \\ &\beta_{\xi_\mu} = 1/2 + \xi_\mu \mu + \nu - \lambda, \ \gamma_{\xi_\mu} = 1 + 2\xi_\mu \mu, \end{aligned}$$

which have hypergeometric functions $F(\alpha, \beta; \gamma; z)$ as solutions; see [1, 20, 81] and the appendix to Sect. 8.7.

Solutions of (8.172) can be obtained from solutions of the latter equations by the transformation (8.173).

The first pair of solutions of (8.172), which we are going to use for constructing Green's functions, are solutions $u_i(x; W)$, $i = 1, 2$,

$$\begin{aligned} u_1(x; \nu) &= \frac{\mathrm{e}^{-i\pi(1/4 + \nu/2)}}{2\pi\mu} \left[\frac{\mathrm{e}^{-i\pi\mu} \Gamma(\gamma_2) P_+(x; W)}{\Gamma(\alpha_2)\Gamma(\beta_2)} - \frac{\mathrm{e}^{i\pi\mu} \Gamma(\gamma_1) P_-(x; W)}{\Gamma(\alpha_1)\Gamma(\beta_1)} \right], \\ u_2(x; W) &= \frac{\mathrm{e}^{i\pi(1/4 + \nu/2)}}{2\pi\mu} \left[\frac{\mathrm{e}^{i\pi\mu} \Gamma(\gamma_2) P_+(x; W)}{\Gamma(\alpha_2)\Gamma(\beta_2)} - \frac{\mathrm{e}^{-i\pi\mu} \Gamma(\gamma_1) P_-(x; W)}{\Gamma(\alpha_1)\Gamma(\beta_1)} \right], \\ u_i(x; W) &= u_i(x; W)|_{\mu \to -\mu}, \ u_i(x; W) = u_i(x; W)|_{\lambda \to -\lambda}, \ i = 1, 2. \end{aligned}$$

The last of these relations means that $u_i(x;W)$ are entire functions of parameters g_1 and g_2. Here auxiliary solutions P_{ξ_μ} and parameters have the form

$$\begin{aligned}
&P_+(x;W) = (-z)^{1/4+\mu}(1-z)^\nu \mathcal{F}(\alpha_1, \beta_{1_\nu}; \gamma_1; z),\ \gamma_{1,2} = \gamma_{+,-} = 1 \pm 2\mu,\\
&P_-(x;W) = (-z)^{1/4-\mu}(1-z)^\nu \mathcal{F}(\alpha_2, \beta_{2_\nu}; \gamma_2; z),\\
&\qquad \alpha_{1,2} = \alpha_{+,-} = 1/2 \pm \mu + \nu + \lambda,\ \beta_{1,2} = \beta_{+,-} = 1/2 \pm \mu + \nu - \lambda,
\end{aligned}$$

where $\mathcal{F}(\alpha, \beta; \gamma; z)$ is an analytic extension of the hypergeometric series in the complex plane $\mathbb{C}$ with a cut along the real $x > 1$ semiaxis given by the Barnes integral; see, e.g., [164].

Using identity (8.115), we find that $P_{\xi_\mu} = P_{\xi_\mu}\big|_{\nu \to -\nu}$, and therefore $u_i(x;W)$ are entire functions in W. We note also that the functions P_{ξ_μ} are analytic in z in the complex plane with a cut along the real positive semiaxis, so that the circle $|z| = 1$ is situated in the analyticity domain of the functions P_{ξ_μ}.

Using (8.117) and (8.115), we obtain another representations for $u_i(x;W)$:

$$u_1(x;W) = \begin{cases} D_2(-z_1)^{1/4+\mu}(1-z)^\nu \mathcal{F}(\alpha_1, \beta_1; \gamma_3; 1-z) \\ +D_3(-z)^{1/4+\mu}(1-z)^{-\nu} \mathcal{F}(\alpha_3, \beta_3; \gamma_4; 1-z),\ \operatorname{Im} z \geq +0, \\ C_1(-z)^{1/4+\mu}(1-z)^\nu \mathcal{F}(\alpha_1, \beta_1; \gamma_3; 1-z),\ \operatorname{Im} z \leq -0, \end{cases}$$

$$u_2(x;W) = \begin{cases} D_1(-z)^{1/4+\mu}(1-z)^\nu \mathcal{F}(\alpha_1, \beta_1; \gamma_3; 1-z),\ \operatorname{Im} z \geq +0, \\ C_2(-z_1)^{1/4+\mu}(1-z)^\nu \mathcal{F}(\alpha_1, \beta_1; \gamma_3; 1-z) \\ +C_3(-z)^{1/4+\mu}(1-z)^{-\nu} \mathcal{F}(\alpha_3, \beta_3; \gamma_4; 1-z),\ \operatorname{Im} z \leq -0, \end{cases} \tag{8.174}$$

where

$$\begin{aligned}
&C_1 = -\frac{e^{-i\pi(1/4+\mu+\nu/2)}}{\pi\Gamma(\gamma_3)},\ D_2 = C_1\left[1 + 2i e^{2i\pi\mu}\frac{\sin(\pi\alpha_1)\sin(\pi\beta_1)}{\sin(\pi\gamma_3)}\right],\\
&D_3 = -2iB^{-1}\Gamma(2\nu)e^{-i\pi(1/4-\mu+\nu/2)},\ B = \Gamma(\alpha_1)\Gamma(\beta_1)\Gamma(\alpha_2)\Gamma(\beta_2),\\
&D_1 = -\frac{e^{i\pi(1/4+\mu+\nu/2)}}{\pi\Gamma(\gamma_3)},\ C_2 = D_1\left[1 - 2i e^{-2i\pi\mu}\frac{\sin(\pi\alpha_1)\sin(\pi\beta_1)}{\sin(\pi\gamma_3)}\right],\\
&C_3 = 2iB^{-1}\Gamma(2\nu)e^{i\pi(1/4-\mu+\nu/2)},\\
&\alpha_3 = 1/2 + \mu - \nu + \lambda,\ \beta_3 = 1/2 + \mu - \nu - \lambda,\ \gamma_{3,4} = 1 \pm 2\nu.
\end{aligned}$$

Representations (8.174) are useful for obtaining asymptotics of the functions u_i as $x \to \pm\infty$.

It is easy to verify that $\overline{u_i(x;\nu)} = u_i(x;\overline{\nu})$, so that $u_i(x;\nu)$ are real for real ν (for $W = E < 0$). In addition, the functions $u_i(x;\nu)$ are analytic in W for $\operatorname{Im} W \neq 0$.

Another pair of solutions of (8.172) that we are going to use is $V_k(x;W)$, $k = 1, 2$,

$$V_1(x;W) = \omega^{-1}(W)[u_1'(0;W)u_2(x;W) - u_2'(0;W)u_1(x;W)],$$
$$V_2(x;W) = \omega^{-1}(W)[u_2(0;W)u_1(x;W) - u_1(0;W)u_2(x;W)],$$
$$u_1(x;W) = u_1(0;W)V_1(x;W) + u_1'(0;W)V_2(x;W),$$

where $\omega(W) = -\mathrm{Wr}(u_1, u_2) \neq 0$. These solutions are normalized, $V_k^{(l-1)}(0;W) = \delta_{kl}$, $k, l = 1, 2$, and are independent, $\mathrm{Wr}(V_1, V_2) = 1$.

As $x \to -\infty$, $\upsilon = \mathrm{e}^{-c|x|} \to 0$, we have

$$z = 1 - 4i\upsilon + O(\upsilon^2),\ -z = \mathrm{e}^{i\pi} + O(\upsilon),\ 1 - z = 4\upsilon\mathrm{e}^{i\pi/2} + O(\upsilon^2),$$
$$u_1(x;W) = -\left[\pi\Gamma(\gamma_3)\right]^{-1}(4\mathrm{e}^{-c|x|})^{\nu}\tilde{O}(\upsilon) \to 0,$$
$$u_2(x;W) = -2B^{-1}\Gamma(2\nu)(\mathrm{e}^{c|x|}/4)^{\nu}\tilde{O}(\upsilon) \to \infty,$$

and as $x \to \infty$, $\upsilon = \mathrm{e}^{cx} \to \infty$

$$z = 1 + 4i/\upsilon + O(\upsilon^{-2}),\ -z = \mathrm{e}^{-i\pi} + O(\upsilon^{-1}),\ 1 - z = (4/\upsilon)\mathrm{e}^{-i\pi/2} + O(\upsilon^2),$$
$$u_1(x;W) = -2B^{-1}\Gamma(2\nu)(\upsilon/4)^{\nu}\tilde{O}(\upsilon^{-1}) \to \infty,$$
$$u_2(x;W) = -\left[\pi\Gamma(\gamma_3)\right]^{-1}(4/\upsilon)^{\nu}\tilde{O}(\upsilon^{-1}) \to 0.$$

Using the above asymptotics, we obtain

$$\mathrm{Wr}(u_1, u_2) = -\frac{2c}{\pi B} = -\omega(W) \neq 0, \infty,\ \operatorname{Im} W > 0,$$

whence it follows that (8.172) has no square-integrable solutions for $\operatorname{Im} W > 0$. That is why the initial symmetric operator $\hat{H}$ defined on the domain $\mathcal{D}(\mathbb{R})$ has zero deficiency indices. In addition, the potential (8.171) tends to zero as $|x| \to \infty$, so that $\Delta_{H^+}(\psi_*) = 0$, as follows from Theorem 7.1. All this implies that the adjoint $\hat{H}^+$ defined on the domain $D^*_{\check{H}}(\mathbb{R})$ is s.a., and $\hat{H}_1 = \hat{H}^+$ is a unique s.a. extension of $\hat{H}$.

As a set of guiding functionals, we can choose

$$\Phi_k(\xi;W) = \int_{-\infty}^{\infty} \mathrm{d}x\, V_k(x;W)\,\xi(x),\ \ \xi \in \mathcal{D}(\mathbb{R}) \cap D^*_{\check{H}}(\mathbb{R}).$$

Following Sect. 5.3.2, we obtain the Green's function of $\hat{H}_1$ and the matrix $M_{kl}(0;W)$,

$$G(x,y;W) = \omega^{-1}(W)\begin{cases} u_2(x;W)u_1(y;W),\ x > y, \\ u_1(x;W)u_2(y;W),\ x < y, \end{cases}$$
$$M_{kl}(0;W) = \omega^{-1}(W)K_{kl}(W),$$
$$K_{kl}(W) = \begin{pmatrix} u_1(0;W)u_2(0;W) & u_1(0;W)u_2'(0;W) \\ u_1'(0;W)u_2(0;W) & u_1'(0;W)u_2'(0;W) \end{pmatrix}.$$

Then the matrix spectral function reads

$$\sigma'_{kl}(E) = \pi^{-1}\,\mathrm{Im}\,\omega^{-1}(E+i0)K_{kl}(E+i0).$$

For $E \geq 0$, $\nu = -i\sqrt{E/c}$, the functions $K_{kl}(E)$ are finite and $\omega^{-1}(E)$ is finite for $E > 0$. For $E = 0$, the function $\omega^{-1}(E)$ is finite if $\beta_2 \neq -n$ $(\mu + \bar{\mu} \neq n + 1/2, n \in \mathbb{Z}_+)$, so that $\sigma'_{kl}(E)$ is finite. If $\mu + \bar{\mu} = n + 1/2 \Longleftrightarrow n = g$, where

$$g = \sqrt{2g_1 + 2\sqrt{g_1^2 + g_2^2}} - 1/2,$$

we have $\omega^{-1}(W) = O\left(1/\sqrt{W}\right)$ as $W \to 0$, so that $\sigma'_{kl}(E)$ has an integrable singularity. Thus, $\sigma'_{kl}(E) = \pi^{-1}\,\mathrm{Im}\,\omega^{-1}(E)K_{kl}(E)$, and therefore all the points of the semiaxis $E \geq 0$ belong to the continuous spectrum.

For $E = -c^2\tau^2 < 0$, $\tau > 0$, $\nu = \tau$, all the functions $u_1(x;\tau)$, $u_2(x;\tau)$, $K_{kl}(E)$, and $\omega(E)$ are real and finite; $\sigma'_{kl}(E)$ differs from zero only at the points E_n,

$$E_n = -c^2\left(g-n\right)^2, \ \tau_n = g - n, \ n = 0, 1, \ldots, n_{\max},$$

$$n_{\max} = \begin{cases} [g], \ g > [g], \\ [g]-1, \ g = [g], \end{cases}$$

that are solutions of the equation $\omega(E_n) = 0 \Longleftrightarrow \beta_2 = -n$ (at least one negative energy level exists if $4g_2^2 > 1/16 - g_1$).

Then we obtain

$$u_2(x;E_n) = (-1)^n \mathrm{e}^{2\pi\,\mathrm{Im}\,\mu} u_1(x;E_n), \ \mathrm{Im}\,\mu = \sqrt{\frac{1}{2}\left(\sqrt{g_1^2 + g_2^2} - g_1\right)},$$

$$K_{kl}(E_n) = (-1)^n \mathrm{e}^{2\pi\,\mathrm{Im}\,\mu} e_{n,k} \otimes e_{n,l}, \ e_{n,k} = \left(u_1(0;E_n), u_1'(0;E_n)\right),$$

and

$$\sigma'_{kl}(E) = \sum_{n=0}^{n_{\max}} Q_n e_{n,k} \otimes e_{n,l}\,\delta(E - E_n),$$

$$Q_n = \sqrt{\frac{\pi c\tau_n \Gamma(2g+1-n)|\Gamma(\beta_1)|^2 \mathrm{e}^{2\pi\,\mathrm{Im}\,\mu}}{n!}}.$$

Finally, the complete spectrum of $\hat{H}_1$ is given by

$$\mathrm{spec}\,\hat{H}_1 = \mathbb{R}_+ \cup \{E_n, \ n = 0, 1, \ldots, n_{\max}\}.$$

The continuous part of the spectrum is twofold degenerate. The discrete spectrum is simple. The inversion formulas have the form

$$\psi(x) = \sum_{k,l=1,2} \int_{\mathbb{R}_+} \varphi_k(E)\sigma'_{kl}(E)V_l(x;E)\mathrm{d}E + \sum_{n=0}^{n_{\max}} \varphi_n U_n(x), \ \forall\psi \in L^2(\mathbb{R}),$$

$$\varphi_k(E) = \int_{\mathbb{R}} V_k(x;E)\psi(x)\mathrm{d}x, \ \varphi_n = \int_{\mathbb{R}} U_n(x)\psi(x)\mathrm{d}x,$$

$$\int_{\mathbb{R}} |\psi(x)|^2\mathrm{d}x = \sum_{k,l=1,2} \int_{\mathbb{R}+} \overline{\varphi_k(E)}\sigma'_{kl}(E)\varphi_l(E)\mathrm{d}E + \sum_{n=0}^{n_{\max}} |\varphi_n|^2,$$

$$U_n(x) = \sum_{k=1,2} Q_n e_{n,k} V_k(x;E_n) = Q_n u_1(x;E_n).$$

Chapter 9
Dirac Operator with Coulomb Field

9.1 Introduction

It is common knowledge that the complete sets of solutions of the Dirac equation, when used in quantizing the spinor free field, allow an interpretation of the QT of the spinor field in terms of particles and antiparticles; see, for example [139]. The space of quantum states of such a free field is decomposed into sectors with a definite number of particles (the vacuum, one-particle sector, and so on). Each sector is stable under time evolution. A description of the one-particle sector of the free spinor field can be formulated as a relativistic QM in which the Dirac equations play the role of the Schrödinger equation and their solutions are interpreted as wave functions of particles and antiparticles.

In QED (and some other models), the concept of the external electromagnetic field is widely and fruitfully used. It can be considered an approximation in which a "very intensive"part of the electromagnetic field is treated classically and is not subjected to any back reaction of the rest of the system. The Dirac equation with such a field plays an important role in QED with an external field (external background). Of special interest are the cases in which an external field allows an exact solution of the Dirac equation. There are a few such exactly solvable cases of physically interesting external electromagnetic fields; see, for example [13, 146]. They can be classified into groups such that the Dirac equations with fields of each group have a similar interpretation.

The constant uniform magnetic field, the plane-wave field, and their parallel combination form the first group; the fields of this group do not violate vacuum stability (do not create particles from the vacuum). Exact solutions of the Dirac equation with such fields form complete systems and can be used in the quantization procedure, providing a particle interpretation for a quantum spinor field in the corresponding external background. This makes possible the construction of an approximation whereby the interaction with the external field is taken into account exactly, while the interaction with the quantized electromagnetic field is treated perturbatively. Such an approach to QED with external fields of the first group is

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known as the Furry picture; see, for example [62, 139]. In the Furry picture, the state space of the QT of the spinor field with the external fields is decomposed into sectors with a definite number of particles; each sector is stable under the time evolution, which is similar to the zero-external-field case. A description of the one-particle sector also can be formulated as a consistent relativistic QM [65].

A uniform electric field and some other electromagnetic fields violate vacuum stability. A literal application of the above approach to constructing the Furry picture in QED with such fields fails. However, it has been demonstrated that existing exact solutions of the Dirac equation with electric-type fields can be used for describing a variety of quantum effects in such fields, in particular, the electron–positron pair production from vacuum [119]. Moreover, these sets of solutions form a basis for constructing a generalized Furry picture in QED with external fields violating vacuum stability; see [60]. It should be noted that the one-particle sector in such external fields is unstable under time evolution, and therefore, the corresponding QM of a spinning particle cannot, in principle, be constructed.

The Dirac equation with the Coulomb field, and with some additional fields, has always been of particular interest. The Coulomb field is even referred to as a "microscopic external field"to underline its qualitative distinction from the above-mentioned external fields, which are sometimes referred to as "macroscopic"ones. Until recently, the commonly accepted view of this situation in theoretical analysis was the following. The Dirac equation for an electron of charge $-e$ in an external Coulomb field created by a positive pointlike electric charge Ze of a nucleus of atomic number[1] $Z \leq Z_{\mathrm{c}} = \alpha^{-1} = 137$ is solved exactly, has a complete set of solutions, and allows the construction of a relativistic theory of atomic spectra that is in agreement with experiment [28]. This field does not violate vacuum stability, and therefore, the Furry picture can be constructed, and the relativistic QM of the spinning particle in such a Coulomb field exists. As for the Dirac equation with the Coulomb field with $Z > Z_{\mathrm{c}}$, it was considered inconsistent and physically meaningless [8, 45, 133]. One of the standard arguments is that the formula for the lower $1S_{1/2}$ energy level,

$$E_{1s} = mc^2\sqrt{1-(Z\alpha)^2}\,,$$

formally gives imaginary eigenvalues for the Dirac Hamiltonian with $Z > Z_{\mathrm{c}}$. The question of consistency of the Dirac equation with the Coulomb field with $Z > Z_{\mathrm{c}}$ is of fundamental importance. The formulation of QED cannot be considered really complete until an exhaustive answer to this question is given.

Although nuclei of electric charges of such magnitude cannot yet be synthesized,[2] the existing heavy nuclei can imitate the supercritical Coulomb fields at collision. Nuclear forces can hold the colliding nuclei together for $10^{-19}\,\mathrm{s}$

[1] $\alpha = e^2/\hbar c$ is the fine structure constant.

[2] At present, the maximum $Z = 118$.

or more. This time is enough to effectively reproduce the experimental situation whereby the electron experiences the supercritical Coulomb field [82]. Several groups of researchers have attacked the problem of the behavior of the electron in the supercritical Coulomb field; see [82, 166]. The difficulty of the imaginary spectrum in the case of $Z > Z_c$ was attributed to an inadmissible singularity of the supercritical Coulomb field for a relativistic electron.[3] It was believed that this difficulty could be eliminated if a nucleus of some finite radius R were considered. It was shown that in cutting off the Coulomb potential with $Z < 173$ at a radius $R \approx 1.2 \times 10^{-12}$ cm, the Dirac equation has physically meaningful solutions [122]. But even in the presence of the cutoff, another difficulty arises at $Z \approx 173$. Namely, the lower bound state energy descends to the upper boundary $E = -mc^2$ of the lower continuum, and it is generally agreed that in such a situation, the problem can no longer be considered a one-particle one because of the electron–positron pair production, which in particular results in a screening of the Coulomb potential of the nucleus. Probabilities of particle production in heavy-ion collisions were calculated within the framework of this concept [82]. Unfortunately, experimental conditions for verifying the corresponding predictions are unavailable at present.

In this chapter, we return to the problem of consistency of the Dirac equation with the Coulomb field with no cutoff and with arbitrary nucleus charge values (with arbitrary Z). Our point of view is that the above-mentioned difficulties with the spectrum for $Z > Z_c$ do not arise if the Dirac Hamiltonian is correctly defined as an s.a. operator. We present a rigorous treatment of all the aspects of this problem including a complete spectral analysis of the model based on the theory of s.a. extensions of symmetric operators and the Krein method of guiding functionals; see [155]. We show that from a mathematical standpoint, the definition of the Dirac Hamiltonian as an s.a. operator for arbitrary Z presents no problem. Moreover, the transition from the noncritical charge region to the critical one does not lead to qualitative changes in the mathematical description of the system. A specific feature of the overcritical charges is a nonuniqueness of the s.a. Dirac Hamiltonian, but this nonuniqueness is characteristic even for $Z > Z_s = (\sqrt{3}/2)\alpha^{-1} \approx 118.68$. For each $Z \geq Z_s$, there exists a family of s.a. Dirac Hamiltonians parameterized by a finite number of extra parameters (and specified by additional boundary conditions at the origin). The existence of these parameters is a manifestation of a nontrivial physics inside the nucleus. A real spectrum and a complete set of eigenstates can be evaluated for each Hamiltonian, so that a relativistic quantum mechanics for an electron in such a Coulomb field can be constructed.

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[3] An equation for the radial components of wave functions has the form of the nonrelativistic Schrödinger equation with an effective potential with the r^{-2} singularity at the origin, which is associated with a "fall to the center".

9.2 Reduction to the Radial Problem

We consider the Dirac equation for a particle of charge q_1 and mass m moving in an external Coulomb field of a charge q_2; for an electron in a hydrogen-like atom, we have[4] $q_1 = -e, q_2 = Ze, Z \in \mathbb{N}$. We choose the electromagnetic potentials for such a field in the form $A^0 = q_2 r^{-1}, A^k = 0, k = 1, 2, 3$. The Dirac equation with this field, written in the form of the Schrödinger equation (in the Hamiltonian form), is[5]

$$i\frac{\partial\Psi(x)}{\partial t} = \check{H}\Psi(x), \ x = \left(x^0, \mathbf{r}\right), \ \mathbf{r} = \left(x^k, \ k = 1, 2, 3\right), \ x^0 = t,$$

where $\Psi(x) = \{\psi_\alpha(x), \alpha = 1, \ldots, 4\}$ is a bispinor (Dirac spinor) and $\check{H}$ is the *s.a. Dirac differential operation*,

$$\check{H} = \boldsymbol{\alpha}\check{\boldsymbol{p}} + m\beta - qr^{-1} = \begin{pmatrix} m - qr^{-1} & \boldsymbol{\sigma}\check{\boldsymbol{p}} \\ \boldsymbol{\sigma}\check{\boldsymbol{p}} & -m - qr^{-1} \end{pmatrix}, \tag{9.1}$$

$\check{\mathbf{p}} = -i\boldsymbol{\nabla}, \boldsymbol{\nabla} = \left(\partial_x, \ \partial_y, \ \partial_z\right), r = |\mathbf{r}|$, and $q = -q_1 q_2$; for an electron in a hydrogen-like atom, we have $q = Z\alpha$. For brevity, we call the coupling constant q the charge. We restrict ourselves to the case $q > 0$.

In the case under consideration, we deal with the Hilbert space $\mathfrak{H} = \boldsymbol{L}^2\left(\mathbb{R}^3\right)$ of square-integrable Dirac spinors $\Psi(\mathbf{r})$ with the scalar product

$$(\Psi_1, \Psi_2) = \int \mathrm{d}\mathbf{r}\Psi_1^+(\mathbf{r})\Psi_2(\mathbf{r}), \ \mathrm{d}\mathbf{r} = \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3 = r^2\mathrm{d}r\,\mathrm{d}\mu(\theta, \varphi),$$

where $\mathrm{d}\mu = \mathrm{d}\mu(\theta, \varphi) = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$ is the integration measure on the sphere, $0 \le \theta \le \pi, 0 \le \varphi \le 2\pi$. The space $\mathfrak{H}$ has the form

$$\mathfrak{H} = \boldsymbol{L}^2\left(\mathbb{R}^3\right) = \sum_{\alpha=1}^{4}{}^{\oplus}\,\mathfrak{H}_\alpha, \ \ \mathfrak{H}_\alpha = L^2(\mathbb{R}^3).$$

We now take the rotational symmetry into account. The group of rotations in $\mathbb{R}^3$ naturally acts in the Hilbert spaces $L^2\left(\mathbb{R}^3\right)$ and $\boldsymbol{L}^2\left(\mathbb{R}^3\right)$ by unitary operator groups U and $\mathcal{U}$: if $S \in \mathrm{Spin}(3)$, then the corresponding operator U_S is defined by the relationship $(U_S\psi)(\mathbf{r}) = \psi\left(S^{-1}\mathbf{r}\right)$, $\psi \in L^2\left(\mathbb{R}^3\right)$, and $\mathcal{U}_S$ is defined by

[4] $e = 4.803 \times 10^{-10}$ CGSE is the magnitude of the electron charge.

[5] We use bold letters for there-vectors and standard representation for γ-matrices, [29], where $\boldsymbol{\alpha} = \mathrm{antidiag}\,(\boldsymbol{\sigma}, \boldsymbol{\sigma})$, $\beta = \gamma^0 = \mathrm{diag}\,(I, -I)$, $\Sigma = \mathrm{diag}\,(\boldsymbol{\sigma}, \boldsymbol{\sigma})$, and $\boldsymbol{\sigma} = \left(\sigma^1, \sigma^2, \sigma^3\right)$ are the Pauli matrices. We use the notation $\boldsymbol{\sigma}\mathbf{p} = \sigma^k p^k$, $\boldsymbol{\sigma}\mathbf{r} = \sigma^k x^k$, and so on. We set $\hbar = c = 1$ in what follows.

the relationship $(\mathcal{U}_S\Psi)(\mathbf{r}) = \Lambda_S\Psi\left(S^{-1}\mathbf{r}\right)$, $\Psi \in \boldsymbol{L}^2\left(\mathbb{R}^3\right)$; the matrices Λ_S are a unitary bispinor representation of the rotation group Spin(3) with the generators $\Sigma/2=\mathrm{diag}(\boldsymbol{\sigma}/2, \boldsymbol{\sigma}/2)$, the spin angular momentum operators. In addition, we introduce the operators

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \Sigma/2 = \mathrm{diag}\,(\hat{\jmath}, \hat{\jmath})\,,\ \hat{\jmath} = \hat{\mathbf{L}} + \boldsymbol{\sigma}/2,\ \hat{\mathbf{J}}^2,$$
$$\hat{K} = \beta\left[1 + \left(\Sigma\hat{L}\right)\right] = \mathrm{diag}\,(\hat{\varkappa}, -\hat{\varkappa})\,,\ \hat{\varkappa} = 1 + \left(\sigma\hat{\mathbf{L}}\right), \tag{9.2}$$

where the orbital angular momentum operators $\hat{\mathbf{L}} = [\mathbf{r}\times\hat{\mathbf{p}}]$ are generators of the group U, the total angular momentum operators $\hat{\mathbf{J}}$ are generators of the group $\mathcal{U}$, and $\hat{\mathbf{J}}^2$ is the Casimir operator of the group $\mathcal{U}$. The operator $\hat{K}$ is called the spin operator; $\hat{\mathbf{J}}^2$, $\hat{J}_3$, and $\hat{K}$ are mutually commuting operators.

The Hilbert space $\mathfrak{H} = \boldsymbol{L}^2\left(\mathbb{R}^3\right)$ is represented as a direct orthogonal sum,

$$\mathfrak{H} = \sum_{j,\zeta}{}^{\oplus}\,\mathfrak{H}_{j,\zeta},\ j = 1/2, 3/2, \ldots,\ \zeta = \pm 1, \tag{9.3}$$

where

$$\mathfrak{H}_{j,\zeta} = \sum_{M}{}^{\oplus}\,\mathfrak{H}_{j,M,\zeta},\ M = -j, -j+1, \ldots, j, \tag{9.4}$$

of subspaces $\mathfrak{H}_{j,\zeta}$ or $\mathfrak{H}_{j,M,\zeta}$, and any bispinor $\Psi \in \mathfrak{H}$ can be represented as

$$\Psi(\mathbf{r}) = \sum_{j,M,\zeta}\Psi_{j,M,\zeta}(\mathbf{r}),$$

where $\Psi_{j,M,\zeta} \in \mathfrak{H}_{j,M,\zeta}$ are functions of the form

$$\Psi_{j,M,\zeta}(\mathbf{r}) = \frac{1}{r}\begin{pmatrix}\Omega_{j,M,\zeta}(\theta,\varphi)f(r)\\ i\Omega_{j,M,-\zeta}(\theta,\varphi)g(r)\end{pmatrix}, \tag{9.5}$$

$\Omega_{j,M,\zeta}$ are spherical spinors, and $f(r)$ and $g(r)$ are radial functions (the factors r^{-1} and i are introduced for convenience).

We use the following representation for the spherical spinors (see [8]):

$$\Omega_{jM\zeta} = \sqrt{\frac{(j-M)!}{4\pi(j+M)!}}\mathrm{e}^{i(M-1/2)\varphi}\begin{pmatrix}[M-\zeta j-(1+\zeta)/2]P^{M-1/2}_{j+\zeta/2}(u)\\ \mathrm{e}^{i\varphi}P^{M+1/2}_{j+\zeta/2}(u)\end{pmatrix},$$
$$j = 1/2, 3/2, \ldots,\ \ M = -j, -j+1, \ldots, j,\ \zeta = \pm 1,\ u = \cos\theta, \tag{9.6}$$

where the adjoint Legendre functions $P_l^m(u)$ are defined as in [81],

$$P_l^m(u) = \frac{1}{2^l l!}(-1)^m(1-u^2)^{m/2}d_u^{l+m}(u^2-1)^l,$$
$$l \in \mathbb{Z}_+,\ \ m = -l, -l+1, \ldots, l.$$

The spherical spinors are eigenvectors of the operators $\hat{\mathbf{J}}^2$, $\hat{J}_z$ and $\hat{\varkappa}$,

$$\hat{j}^2\Omega_{j,M,\zeta}(\mathbf{r}) = j(j+1)\Omega_{j,M,\zeta}(\mathbf{r}), \ \hat{j}_z\Omega_{j,M,\zeta}(\mathbf{r}) = M\Omega_{j,M,\zeta},$$
$$\hat{\varkappa}\Omega_{j,M,\zeta}(\mathbf{r}) = -\zeta(j+1/2)\Omega_{j,M,\zeta}(\mathbf{r}).$$

These spinors are orthonormalized,

$$\int \Omega^{+}_{j'M'\zeta'}(\theta,\varphi)\Omega_{jM\zeta}(\theta,\varphi)d\mu = \delta_{jj'}\delta_{MM'}\delta_{\zeta\zeta'},$$

and form a complete orthonormal basis in the space of spinors on the sphere.

The bispinors $\Psi_{j,M,\zeta}(\mathbf{r})$ are eigenvectors of the operators $\hat{\mathbf{J}}^2$, $\hat{J}_3$, and $\hat{K}$,

$$\hat{\mathbf{J}}^2\Psi_{j,M,\zeta}(\mathbf{r}) = j(j+1)\Psi_{j,M,\zeta}(\mathbf{r}), \hat{J}_z\Psi_{j,M,\zeta}(\mathbf{r}) = M\Psi_{j,M,\zeta},$$
$$\hat{K}\Psi_{j,M,\zeta}(\mathbf{r}) = -\zeta(j+1/2)\Psi_{j,M,\zeta}(\mathbf{r}).$$

The subspaces $\mathfrak{H}_{j,\zeta}$ reduce[6] the operators $\hat{\mathbf{J}}^2$, $\hat{\mathbf{J}}$, and $\hat{K}$,

$$\hat{\mathbf{J}}^2 = \sum_{j,\zeta}^{\oplus}\hat{\mathbf{J}}^2_{j,\zeta}, \ \hat{\mathbf{J}} = \sum_{j,\zeta}^{\oplus}\hat{\mathbf{J}}_{j,\zeta},$$
$$\hat{K} = \sum_{j,\zeta}^{\oplus}\hat{K}_{j,\zeta},$$

and the subspaces $\mathfrak{H}_{j,M,\zeta}$ reduce the operators $\hat{\mathbf{J}}^2_{j,\zeta}$, $\left(\hat{J}_z\right)_{j,\zeta}$, and $\hat{K}_{j,\zeta}$,

$$\hat{\mathbf{J}}^2_{j,\zeta} = \sum_{M}^{\oplus}\hat{\mathbf{J}}^2_{j,M,\zeta}, \ \left(\hat{J}_z\right)_{j,\zeta} = \sum_{M}^{\oplus}\left(\hat{J}_z\right)_{j,M,\zeta},$$
$$\hat{K}_{j,\zeta} = \sum_{M}^{\oplus}\hat{K}_{j,M,\zeta}.$$

In the language of physics, decompositions (9.3) and (9.4) correspond to an expansion of bispinors $\Psi(\mathbf{r})$ in terms of eigenfunctions of the commuting operators $\hat{\mathbf{J}}^2$, $\hat{J}_z$, and $\hat{K}$, which permits separation of variables in equations for the eigenfunctions.

We note that the reductions $\hat{\mathbf{J}}_{j,\zeta}$ of the operators $\hat{\mathbf{J}}$ to the subspaces $\mathfrak{H}_{j,\zeta}$ are bounded operators.

---

[6]This means that the operators $\hat{\mathbf{J}}^2$, $\hat{J}_3$, and $\hat{K}$ commute with the projectors to the subspaces $\mathcal{H}_{j,\zeta}$; see [9, 116].

Let $\mathbb{L}^2(\mathbb{R}_+)$ be the Hilbert space of doublets $F(r)$,

$$F(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = (f(r)/g(r)),$$

with the scalar product

$$(F_1, F_2) = \int_{\mathbb{R}_+} \mathrm{d}r F_1^+(r) F_2(r) = \int_{\mathbb{R}_+} \mathrm{d}r \left[\overline{f_1(r)} f_2(r) + \overline{g_1(r)} g_2(r)\right],$$

so that $\mathbb{L}^2(\mathbb{R}_+) = L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$.

Then (9.5) and the relation

$$\left\|\Psi_{j,M,\zeta}\right\|^2 = \int_{\mathbb{R}_+} \mathrm{d}r \left[|f(r)|^2 + |g(r)|^2\right]$$

show that $\mathfrak{H}_{j,M,\zeta}$ is isometric to $\mathbb{L}^2(\mathbb{R}_+)$:

$$\Psi_{j,M,\zeta} = S_{j,M,\zeta} F, \ \ F = S^{-1}_{j,M,\zeta} \Psi_{j,M,\zeta}.$$

The explicit form of this isometry is

$$\Psi_{j,M,\zeta}(\mathbf{r}) = r^{-1} \mathbf{\Pi}_{j,M,\zeta}(\theta,\varphi) F(r), \ \ F(r) = r \int \mathrm{d}\mu(\theta,\varphi) \mathbf{\Pi}^+_{j,M,\zeta}(\theta,\varphi) \Psi_{j,M,\zeta}(\mathbf{r}). \tag{9.7}$$

Here $\mathbf{\Pi}_{j,M,\zeta}$ and $\mathbf{\Pi}^+_{j,M,\zeta}$ are respectively (4×2) and (2×4) matrices,

$$\mathbf{\Pi}_{j,M,\zeta} = \begin{pmatrix} \Omega_{j,M,\zeta} & \mathbf{0} \\ \mathbf{0} & i\Omega_{j,M,-\zeta} \end{pmatrix}, \mathbf{\Pi}^+_{j,M,\zeta} = \begin{pmatrix} \Omega^+_{j,M,\zeta} & \mathbf{0}^T \\ \mathbf{0}^T & -i\Omega^+_{j,M,-\zeta} \end{pmatrix},$$

$$\int \mathrm{d}\mu(\theta,\varphi) \left[\mathbf{\Pi}^+_{j,M,\zeta}(\theta,\varphi) \mathbf{\Pi}_{j,M,\zeta}(\theta,\varphi)\right]_{ab} = \delta_{ab}, \quad a, b = 1, 2,$$

where $\mathbf{0} = (0/0)$ is a two-column and $\mathbf{0}^T = (0,0)$ is a two-line.

Now we define a rotationally invariant initial symmetric operator $\hat{H}$ associated with the s.a. differential operation $\check{H}$. Because coefficient functions of $\check{H}$ are smooth away from the origin, we choose the space of smooth bispinors with compact support[7] for the domain D_H of $\hat{H}$. To avoid trouble with the $1/r$ singularity of the potential at the origin, we additionally require that all bispinors in D_H vanish near the origin.[8] The operator $\hat{H}$ is thus defined by

$$\hat{H} = \begin{cases} D_H = \left\{\Psi(\mathbf{r}) : \ \psi_\alpha(\mathbf{r}) \in \mathcal{D}(\mathbb{R}^3) \setminus \{0\}\right\}, \\ \hat{H}\Psi(\mathbf{r}) = \check{H}\Psi(\mathbf{r}), \end{cases}$$

[7] We thus avoid difficulties associated with the behavior of wave functions at infinity.

[8] Strictly speaking, we thus leave room for δ-like terms in the potential.

where $\mathcal{D}(\mathbb{R}^3)\setminus\{0\}$ is the space of smooth functions in $\mathbb{R}^3$ with compact support and vanishing in some neighborhood of the origin. The domain D_H is dense in $\mathfrak{H}$, and the symmetry of $\hat{H}$ is easily verified. The operator $\hat{H}$ evidently commutes with the operators $\hat{\mathbf{J}}^2$, $\hat{\mathbf{J}}$, and $\hat{K}$.

The rotational invariance of $\hat{H}$ is equivalent to the following statements.

(a) The subspaces $\mathfrak{H}_{j,M,\zeta}$ reduce this operator: Let $\Psi(\mathbf{r}) = \sum_{j,M,\zeta}\Psi_{j,M,\zeta}(\mathbf{r})$, $\Psi \in D_H$, and let $P_{j,\zeta}$ and $P_{j,M,\zeta}$ be orthoprojectors on $\mathfrak{H}_{j,\zeta}$ and $\mathfrak{H}_{j,M,\zeta}$ respectively. Then $\Psi_{j,M,\zeta} = P_{j,M,\zeta}\Psi \in D_H$ and $\hat{H}\Psi = \sum_{j,M,\zeta}\hat{H}_{j,M,\zeta}\Psi_{j,M,\zeta}$, where $\hat{H}_{j,M,\zeta} = P_{j,M,\zeta}\hat{H}P_{j,M,\zeta} = \hat{H}P_{j,M,\zeta}$, are parts of $\hat{H}$ acting in subspaces $\mathfrak{H}_{j,M,\zeta}$.
Each $\hat{H}_{j,M,\zeta}$ is a symmetric operator in the subspace $\mathfrak{H}_{j,M,\zeta}$. Each symmetric operator $\hat{H}_{j,M,\zeta}$ in the subspace $\mathfrak{H}_{j,M,\zeta}$ evidently induces a symmetric operator $\hat{h}_{j,M,\zeta}$ in the Hilbert space $\mathbb{L}^2(\mathbb{R}_+)$,

$$\hat{h}_{j,M,\zeta}F = S^{-1}_{j,M,\zeta}\hat{H}_{j,M,\zeta}\Psi_{j,M,\zeta},$$

so that $\hat{h}_{j,M,\zeta} = S^{-1}_{j,M,\zeta}\hat{H}_{j,M,\zeta}S_{j,M,\zeta}$ is given by

$$\hat{h}_{j,M,\zeta} = \begin{cases} D_{h_{j,\zeta}} = \mathfrak{D}(\mathbb{R}_+) = \mathcal{D}(\mathbb{R}_+)\oplus\mathcal{D}(\mathbb{R}_+), \\ \hat{h}_{j,M,\zeta}F(r) = \check{h}_{j,\zeta}F(r), \end{cases} \tag{9.8}$$

and the s.a. differential operation $\check{h}_{j,\zeta}$ reads

$$\check{h}_{j,\zeta} = -i\sigma^2 d_r + \varkappa r^{-1}\sigma^1 - qr^{-1} + m\sigma^3,\ \ \varkappa = \zeta(j+1/2). \tag{9.9}$$

(b) The differential operation $\check{h}_{j,\zeta}$, and consequently, taking (9.8) into account, the operator $\hat{h}_{j,M,\zeta}$ with fixed j and ζ, are independent of M, that is, $\hat{h}_{j,M,\zeta} = \hat{h}_{j,\zeta}$. This fact is equivalent to the commutativity of the operator $\hat{H}_{j,\zeta} = P_{j,\zeta}\hat{H}P_{j,\zeta} = \hat{H}P_{j,\zeta}$ with the operators $(\hat{J}_{x,y})_{j,\zeta}$.

In what follows, while on the subject of the *rotational invariance* of any (closed) operator $\hat{f}$, we suppose that the following properties hold:

(1) The reducibility of $\hat{f}$ by the subspaces $\mathfrak{H}_{j,M,\zeta}$ and therefore by $\mathfrak{H}_{j,\zeta}$, so that the operator $\hat{f}$ can be represented in the form

$$\hat{f} = \sum_{j,\zeta}{}^{\oplus}\hat{f}_{j,\zeta} = \sum_{j,M,\zeta}{}^{\oplus}\hat{f}_{j,M,\zeta},$$

$$\hat{f}_{j,\zeta} = P_{j,\zeta}\hat{f}P_{j,\zeta} = \hat{f}P_{j,\zeta},\ \ \hat{f}_{j,M,\zeta} = P_{j,M,\zeta}\hat{f}P_{j,M,\zeta} = \hat{f}P_{j,M,\zeta}.$$

(2) The commutativity of the operators $\hat{f}_{j,\zeta}$ with the bounded operators $\hat{J}^{1,2}_{j,\zeta}$ for any j and ζ.

Let $(\hat{h}_{j,\zeta})_{\mathfrak{e}}$ be an s.a. extension of $\hat{h}_{j,\zeta}$ in $\mathbb{L}^2(\mathbb{R}_+)$, an *s.a. radial Hamiltonian*. It evidently induces s.a. extensions $(\hat{H}_{j,M,\zeta})_{\mathfrak{e}}$ of the symmetric operators $\hat{H}_{j,M,\zeta}$ in the subspaces $\mathfrak{H}_{j,M,\zeta}$,

$$(\hat{H}_{j,M,\zeta})_{\mathfrak{e}} = S_{j,M,\zeta}(\hat{h}_{j,\zeta})_{\mathfrak{e}} S^{-1}_{j,M,\zeta},$$

and the operator $(\hat{H}_{j,\zeta})_{\mathfrak{e}} = \sum^{\oplus}_{M} (\hat{H}_{j,M,\zeta})_{\mathfrak{e}}$ commutes with $\hat{J}^{1,2}_{j,\zeta}$. Then the direct orthogonal sum of the operators $\left(\hat{H}_{j,\zeta}\right)_{\mathfrak{e}}$ is an s.a. operator $\hat{H}_{\mathfrak{e}}$,

$$\hat{H}_{\mathfrak{e}} = \sum_{j,\zeta}{}^{\oplus} (\hat{H}_{j,\zeta})_{\mathfrak{e}}, \tag{9.10}$$

in the whole Hilbert space $\mathfrak{H}$ (see [125]). Thus, $\hat{H}_{\mathfrak{e}}$ is a rotationally invariant extension of the rotationally invariant initial symmetric operator $\hat{H}$ (an *s.a. Dirac Hamiltonian*).

Conversely, any rotationally invariant s.a. extension of the initial operator $\hat{H}$ has structure (9.10), and the operator $(\hat{h}_{j,\zeta})_{\mathfrak{e}} = S^{-1}_{j,M,\zeta}(\hat{H}_{j,M,\zeta})_{\mathfrak{e}} S_{j,M,\zeta}$ in $\mathbb{L}^2(\mathbb{R}_+)$ is independent of M and is an s.a. extension of the symmetric operator[9] $\hat{h}_{j,\zeta}$.

The problem of constructing a rotationally invariant s.a. Dirac Hamiltonian $\hat{H}_{\mathfrak{e}}$ is thus reduced to the problem of constructing s.a. radial Hamiltonians $(\hat{h}_{j,\zeta})_{\mathfrak{e}}$.

In what follows, we consider fixed j and ζ and therefore omit these indices for brevity. In fact, we consider the radial differential operations $\check{h}_{j,\zeta}$ as a two-parameter differential operation $\check{h}$ with the parameters q and $\varkappa$ (the parameters j and ζ enter through the one parameter $\varkappa$, the parameter m is considered fixed) and similarly treat the associated radial operators $\hat{h}$ and $\hat{h}_{\mathfrak{e}}$ defined in the same Hilbert space $\mathbb{L}^2(\mathbb{R}_+)$.

9.3 Solutions of Radial Equations

Below, we consider the differential equation $\check{h}F = WF$ with an arbitrary complex W; real W are denoted by E and have the conventional sense of energy. This equation for the doublet $F = (f\,/\,g)$ is equivalent to a set of *radial equations* for $f(r)$ and $g(r)$,

[9]Roughly speaking, this means that s.a. extensions of the parts $\hat{H}_{j,M,\zeta}$ with fixed j and ζ and different M's must be constructed "uniformly".

$$
\begin{aligned}
&f' + \varkappa r^{-1} f - \left(W + m + qr^{-1}\right) g = 0, \\
&g' - \varkappa r^{-1} g + \left(W - m + qr^{-1}\right) f = 0.
\end{aligned} \tag{9.11}
$$

We note that the Wronskian of the doublets $F_1 = (f_1 / g_1)$ and $F_2 = (f_2 / g_2)$ reads $\mathrm{Wr}\,(F_1, F_2) = f_1 g_2 - g_1 f_2$.

We present the general solution of the radial equations following the standard procedure; see, for example [8, 133]. We first represent $f(r)$ and $g(r)$ as

$$
f(r) = z^{\Upsilon} \mathrm{e}^{-z/2} \left[Q(z) + P(z)\right], \; g(r) = i\Lambda z^{\Upsilon} \mathrm{e}^{-z/2} \left[Q(z) - P(z)\right],
$$

where

$$
\begin{aligned}
&z = -2iKr, \; \Lambda = \sqrt{\frac{W-m}{W+m}}, \; W \pm m = \rho_{\pm} \mathrm{e}^{i\varphi_{\pm}}, \; 0 \le \varphi_{\pm} < \pi, \\
&\Lambda = \sqrt{\rho_-/\rho_+} \mathrm{e}^{\frac{i}{2}(\varphi_- - \varphi_+)}, \; K = \sqrt{W^2 - m^2} = \sqrt{\rho_- \rho_+} \mathrm{e}^{\frac{i}{2}(\varphi_- + \varphi_+)},
\end{aligned}
$$

and Υ obeys the condition $\Upsilon^2 = \varkappa^2 - q^2$. Radial equations (9.11) then become equations for the functions P and Q,

$$
\begin{aligned}
&zQ'' + (\beta - z)\, Q' - \alpha Q = 0, \; \beta = 1 + 2\Upsilon, \; \alpha = \alpha_+, \\
&P = -b_+^{-1} \left(z d_z + \alpha\right) Q, \; b_{\pm} = \varkappa \pm qm(iK)^{-1}, \; \alpha_{\pm} = \Upsilon \pm qW(iK)^{-1}.
\end{aligned} \tag{9.12}
$$

The first equation in (9.12) is the confluent hypergeometric equation for Q; see [1, 20, 81].

Let[10] $\Upsilon \neq -n/2, n \in \mathbb{N}$. Then the general solution for Q can be represented as

$$
Q = A\Phi(\alpha, \beta; z) + B\Psi(\alpha, \beta; z)\,, \tag{9.13}
$$

where A and B are arbitrary constants; $\Phi(\alpha, \beta; z)$ and $\Psi(\alpha, \beta; z)$ are the known confluent hypergeometric functions (the function $\Phi(\alpha, \beta; z)$ is not defined for $\beta \in \mathbb{Z}_-$).

It follows from (9.12) and (9.13) that

$$
P = -Aa\Phi(\alpha + 1, \beta; z) + Bb_- \Psi(\alpha + 1; \beta; z)\,, \; a = \alpha_+ b_+^{-1}.
$$

Then the general solution of radial equations (9.11) for any complex W and real m, $\varkappa$, and q is finally given by

[10] The parameter Υ is defined up to a sign. The specification of Υ is a matter of convenience. In particular, for specific values of charge, we also use a specification of Υ where $\Upsilon = -n/2$; this case is considered separately below.

$$\begin{aligned} f(r) &= z^{\Upsilon} \mathrm{e}^{-z/2} \{A\,[\Phi(\alpha,\beta;z) - a\Phi(\alpha+1,\beta;z)] \\ &\quad + B\,[\Psi(\alpha,\beta;z) + b_-\Psi(\alpha+1;\beta;z)]\}\,, \\ g(r) &= i\Lambda z^{\Upsilon} \mathrm{e}^{-z/2} \{A[\Phi(\alpha,\beta;z) + a\Phi(\alpha+1,\beta;z)] \\ &\quad + B\,[\Psi(\alpha,\beta;z) - b_-\Psi(\alpha+1;\beta;z)]\}\,. \end{aligned}$$

Taking the relationship

$$\Phi(\alpha+1,\beta;-2iKr) = \mathrm{e}^{-2iKr}\Phi(\beta-\alpha-1,\beta;2iKr)$$

into account (see [1, 20, 81]), it is convenient to represent the general solution of radial equations (9.11) in the form

$$F = AX(r,\Upsilon,W) + Bz^{\Upsilon}\mathrm{e}^{-z/2}\,[\Psi(\alpha,\beta;z)\varrho_+ - b_-\Psi(\alpha+1,\beta;z)\varrho_-]\,, \quad (9.14)$$

where $\varrho_\pm = (\pm 1 \diagup i\Lambda)$ and doublets X are defined as

$$\begin{aligned} X &= \frac{(2\mathrm{e}^{-i\pi/2}K/m)^{-\Upsilon}}{2(1-a_+)} z^{\Upsilon}\mathrm{e}^{-z/2}[\Phi(\alpha,\beta;z) - a\Phi(\alpha+1,\beta;z)] \\ &= \frac{(mr)^{\Upsilon}}{2}\,[\Phi_+(r,\Upsilon,W) + \Phi_-(r,\Upsilon,W)\Xi]\,d_+, \\ \Phi_+ &= \mathrm{e}^{iKr}\Phi\,(\alpha,1+2\Upsilon;-2iKr) + \mathrm{e}^{-iKr}\Phi\,(\alpha_-,1+2\Upsilon;2iKr), \\ \Phi_- &= (iK)^{-1}\left[\mathrm{e}^{iKr}\Phi\,(\alpha,1+2\Upsilon;-2iKr) - \mathrm{e}^{-iKr}\Phi\,(\alpha_-,1+2\Upsilon;2iKr)\right], \\ d_\pm &= \left(1 \diagup (\varkappa \pm \Upsilon)\,q^{-1}\right); \end{aligned} \quad (9.15)$$

the doublet d_- will be used below, and $\Xi = \operatorname{antidiag}(m-W, m+W)$.

We now present some particular solutions of radial equations (9.11) that are used in the following.

One of the solutions given by (9.14) with $A = 1$, $B = 0$, and a specific choice of Υ reads

$$\begin{aligned} F_1(r;W) &= X(r,\Upsilon_+,W), \quad \Upsilon_+ = \begin{cases} \gamma, & q \le |\varkappa|, \\ i\sigma, & q > |\varkappa|, \end{cases} \\ \gamma &= \sqrt{\varkappa^2 - q^2} \ge 0,\ q \le |\varkappa|;\ \sigma = \sqrt{q^2 - \varkappa^2} > 0,\ q > |\varkappa|. \end{aligned} \quad (9.16)$$

The asymptotic behavior of the doublet $F_1(r;W)$ at the origin is given by

$$F_1(r;W) = (mr)^{\Upsilon_+}d_+ + O(r^{\Upsilon_+ + 1}),\ r \to 0.$$

In the case $\Upsilon_+ \neq n/2, n \in \mathbb{N}$, we also use another solution,

$$F_2(r; W) = X(r, -\Upsilon_+, W), \tag{9.17}$$

with the asymptotic behavior

$$F_2(r; W) = (mr)^{-\Upsilon_+} d_- + O(r^{-\Upsilon_+ +1}),\ r \to 0. \tag{9.18}$$

It is useful to introduce the function $q_c(j)$,

$$q_c(j) = |\varkappa| = j + 1/2. \tag{9.19}$$

For $q = q_c(j)$, we have $\Upsilon_+ = 0$. For $q \neq q_c(j)$, that is, for $\Upsilon_+ \neq 0$, the solutions F_1 and F_2 are linearly independent, $\mathrm{Wr}\,(F_1, F_2) = -2\Upsilon_+ q^{-1}$.

It follows from the standard representation for Φ that for real Υ, ($\Upsilon \neq -n/2$), the functions Φ_+ and Φ_- in (9.15) are real entire in W. It then follows from (9.16) and (9.17) that the respective doublets $F_1(r; W)$ and $F_2(r; W)$ are also real entire in W for real $\Upsilon_+ = \gamma$. If Υ_+ is pure imaginary, $\Upsilon_+ = i\sigma$, then F_1 and F_2 are entire in W and are complex conjugate for real $W = E$, $\overline{F_1(r; E)} = F_2(r; E)$.

Another useful solution $F_3(r; W)$ nontrivial for $\Upsilon_+ \neq n/2, n \in \mathbb{N}$, is given by (9.14) with $A = 0$ and a special choice for B:

$$\begin{aligned} F_3(r; W) &= B(W) z^{\Upsilon_+} \mathrm{e}^{iKr} \left[\Psi(\alpha, \beta; z)\varrho_+ - b_- \Psi(\alpha + 1; \beta; z)\, \varrho_-\right], \\ B(W) &= \frac{1}{2}\Gamma(-\alpha_-)\left(1 + \frac{(m + W)(\varkappa + \Upsilon_+)}{iqK}\right)\left(2\mathrm{e}^{-i\pi/2} K/m\right)^{-\Upsilon_+}. \end{aligned} \tag{9.20}$$

Like any solution, F_3 is a linear combination of F_1 and F_2,

$$F_3 = \Gamma(-2\Upsilon_+) F_1 + q\,(2\Upsilon_+)^{-1}\,\omega(W) F_2,\ \omega(W) = -\mathrm{Wr}\,(F_1, F_3), \tag{9.21}$$

where

$$\omega = \frac{\Gamma(1 + 2\Upsilon_+)\Gamma(-\alpha_-)[iqK + (\varkappa + \gamma)(W + m)](2\mathrm{e}^{-i\pi/2} K/m)^{-2\Upsilon_+}}{q\Gamma(\alpha)[iqK + (\varkappa - \gamma)(W + m)]}. \tag{9.22}$$

We note that if $\mathrm{Im}\, W > 0$ and $r \to \infty$, the doublet F_1 increases exponentially, while F_3 decreases exponentially (with polynomial accuracy).

Consider the special case of $q = q_c(j)$ ($\Upsilon_+ = 0$), where the doublets F_1 and F_2 coincide.

Differentiating radial equations (9.11) with respect to γ at $\gamma = 0$, we can easily verify that the doublet

$$\partial_\gamma F_1(r; W)\big|_{\gamma=0} = \lim_{\gamma \to 0} [F_1(r; W) - F_2(r; W)]\,(2\gamma)^{-1}$$

is a solution of these equations with $\gamma = 0$. For two linearly independent solutions of radial equations (9.11) with $\gamma = 0$, we choose

$$
\begin{aligned}
F_1^{(0)}(r; W) &= F_1(r; W)\big|_{\gamma=0},\\
F_1^{(0)}(r; W) &= d_+ + O(r),\ r \to 0,\\
F_2^{(0)}(r; W) &= \partial_\gamma F_1(r; W)\big|_{\gamma=0} - \zeta q_c^{-1}(j)\, F_1^{(0)}(r; W),\\
F_2^{(0)}(r; W) &= d_0(r) + O(r \ln r),\ r \to 0;\\
d_+\big|_{\gamma=0} &= (1 \diagup \zeta),\\
d_0(r) &= \big(\ln(mr) - \zeta q_c^{-1}(j) \diagup \zeta \ln(mr)\big).
\end{aligned} \tag{9.23}
$$

Both solutions $F_1^{(0)}$ and $F_2^{(0)}$ are real entire in W and independent, $\mathrm{Wr}(F_1^{(0)}, F_2^{(0)}) = q_c^{-1}(j)$.

As an analogue of F_3 in the case of $\gamma = 0$, we take the doublet $F_3^{(0)}$,

$$
\begin{aligned}
F_3^{(0)} &= -\lim_{\gamma \to 0} F_3 = -(1 - a_0)^{-1}\, \Gamma(\alpha_0) \mathrm{e}^{iKr}\\
&\quad \times \left[\Psi(\alpha_0, 1; -2iKr) + b_0 \Psi(\alpha_0 + 1, 1; -2iKr)\, \sigma^3\right] \varrho_+,\\
\alpha_0 &= -iq_c(j)\, WK^{-1},\ a_0 = W(m + i\zeta K)^{-1},\\
b_0 &= q_c(j)\, K^{-1}(\zeta K + im).
\end{aligned} \tag{9.24}
$$

Its representation in terms of $F_1^{(0)}$ and $F_2^{(0)}$ is given by

$$
\begin{aligned}
F_3^{(0)} &= F_2^{(0)} + f F_1^{(0)},\ \mathrm{Wr}\left(F_2^{(0)}, F_3^{(0)}\right) = -\omega^{(0)},\ \omega^{(0)} = \omega^{(0)}(W),\\
f &= f(W) = q_c(j)\, \omega^{(0)}(W) = \ln\left(2\mathrm{e}^{-i\pi/2} K/m\right) + \psi\left(-iq_c(j)\, WK^{-1}\right)\\
&\quad + (\zeta(W - m) + iK)\, (2q_c(j)\, W)^{-1} - 2\psi(1),
\end{aligned}
$$

where $\psi(x) = \Gamma'(x)\Gamma^{-1}(x)$.

We note that for $\mathrm{Im}\, W > 0$, the doublet $F_3^{(0)}$ is square-integrable on the semiaxis $\mathbb{R}_+$, that is, $F_3^{(0)} \in \mathbb{L}^2(\mathbb{R}_+)$.

9.4 Self-adjoint Radial Hamiltonians

9.4.1 Generalities

Here we are going to construct s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}$ in the Hilbert space $\mathbb{L}^2(\mathbb{R}_+)$ as s.a. extensions of the initial symmetric radial operators $\hat{h}$ (9.8) associated with the radial differential operations $\check{h}$ (9.9) and analyze the corresponding spectral problems. We note that the result crucially depends on the value of the charge q. Therefore, our exposition is naturally divided into subsections related to the corresponding regions of the charge; there are four of them.

In what follows, all the operators associated to the differential operation $\check{h}$ act on their domains as $\check{h}$, so that we will indicate only these domains.

We begin with the adjoint $\hat{h}^+$ of the initial symmetric operator $\hat{h}$. Its domain D_{h^+} is the natural domain for $\check{h}$,

$$D_{h^+} = D^*_{\check{h}}(\mathbb{R}_+) = \left\{F_* : \; F_* \text{ a.c. in } \mathbb{R}_+, \; F_*, \check{h}F_* \in \mathbb{L}^2(\mathbb{R}_+)\right\}.$$

In the case under consideration, the quadratic asymmetry form $\varDelta_{h^+}(F_*)$ is expressed in terms of the local quadratic form $[F_*, F_*](r)$ as follows:

$$\begin{aligned}
\varDelta_{h^+}(F_*) &= \left(F_*, \hat{h}^+F_*\right) - \left(\hat{h}^+F_*, F_*\right) = [F, F](r)|_0^\infty, \\
[F_*, F_*](r) &= \overline{g(r)}f(r) - \overline{f(r)}g(r), \quad F_* = (f / g).
\end{aligned} \tag{9.25}$$

One can prove that

$$\lim_{r\to\infty} F_*(r) = 0, \quad \forall F_* \in D^*_{\check{h}}(\mathbb{R}_+). \tag{9.26}$$

To this end, we first note that $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$ implies that $G = \check{h}F_*$ is square-integrable together with F_*. It then follows that

$$F_*'(r) = \left(-\varkappa r^{-1}\sigma^3 + iqr^{-1}\sigma^2 + m\sigma^1\right)F_*(r) + i\sigma^2 G(r)$$

is square-integrable at infinity.

It now remains for us to refer to the assertion that if an a.c. $F(r)$ is square-integrable at infinity together with its derivative $F'(r)$, then $F(r) \overset{r\to\infty}{\longrightarrow} 0$; this assertion is an evident generalization of a similar assertion for scalar functions; see Lemma 2.13. Therefore, the boundary form $[F_*, F_*](\infty)$ is identically zero and the asymmetry form $\varDelta_{h^+}(F_*)$ is determined by the boundary form $[F_*, F_*](0)$ at the origin.

A result of constructing s.a. radial Hamiltonians $\hat{h}$ essentially depends on the values of the parameters Z and j. There are two regions in the first quadrant j, Z, we call them nonsingular and singular ones, where the problem of s.a. extensions has principally different solutions. These regions are separated by the singular curve $Z = Z_{\mathrm{s}}(j)$, where

$$Z_{\mathrm{s}}(j) = \sqrt{j(j+1)}\alpha^{-1}$$

such that the nonsingular and singular regions are defined by the respective inequalities $Z \le Z_{\mathrm{s}}(j)$ and $Z > Z_{\mathrm{s}}(j)$. The value $Z_{\mathrm{s}}(j) = 118.68, 265.37, \ldots$ can be called the singular Z-value for a given j. Below, we consider s.a. radial Hamiltonians $\hat{h}$ and their spectra in the nonsingular and singular regions separately.

For the evaluation of the asymptotic behavior of $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$ at the origin, the doublets F_* can be considered square-integrable solutions of the inhomogeneous differential equation

$$\check{h}F_*(r) = G(r),\ G \in \mathbb{L}^2(\mathbb{R}_+). \tag{9.27}$$

It is convenient to represent (9.27) as follows:

$$\begin{aligned}
&\check{h}_- F_*(r) = G_-(r) \in \mathbb{L}^2(\mathbb{R}_+),\\
&\check{h}_- = -i\sigma^2 d_r + \varkappa r^{-1}\sigma^1 - qr^{-1}, G_-(r) = G(r) - m\sigma^3 F_*(r)\,.
\end{aligned}$$

Let u_1 and u_2 be linearly independent solutions of the equation $\check{h}_- u = 0$,

$$\begin{aligned}
&u_1(r) = (mr)^{\Upsilon_+} d_+\,,\ q > 0,\\
&u_2(r) = \begin{cases} (mr)^{-\Upsilon_+} d_-\,,\ q > 0,\ q \ne q_{\mathrm{c}}(j)\,,\\ d_0(r),\ q = q_{\mathrm{c}}(j)\,. \end{cases}
\end{aligned} \tag{9.28}$$

Any solution $F_*(r)$ of (9.27) can be represented as

$$F_*(r) = c_1 u_1(r) + c_2 u_2(r) + I_1(r) + I_2(r), \tag{9.29}$$

where c_1 and c_2 are some constants and

$$\begin{aligned}
&I_1(r) = \begin{cases} (q/2\Upsilon_+)\int_r^{r_0}[u_1(r)\otimes u_2(y)]G_-(y)\mathrm{d}y,\ 0 < q \le q_{\mathrm{s}}(j),\\ -(q/2\Upsilon_+)\int_0^r[u_1(r)\otimes u_2(y)]G_-(y)\mathrm{d}y,\ q > q_{\mathrm{s}}(j)\,,\ q \ne q_{\mathrm{c}}(j),\\ q_{\mathrm{c}}(j)\int_0^r[u_1(r)\otimes u_2(y)]G_-(y)\mathrm{d}y,\ q = q_{\mathrm{c}}(j), \end{cases}\\
&I_2(r) = \begin{cases} (q/2\Upsilon_+)\int_0^r[u_2(r)\otimes u_1(y)]G_-(y)\mathrm{d}y,\ q > 0,\ q \ne q_{\mathrm{c}}(j)\,,\\ -q_{\mathrm{c}}(j)\int_0^r[u_2(r)\otimes u_1(y)]G_-(y)\mathrm{d}y,\ q = q_{\mathrm{c}}(j)\,. \end{cases}
\end{aligned}$$

Here $r_0 > 0$ is a constant, and $\otimes$ is the symbol of the tensor product, so that $[u_1(r)\otimes u_2(y)]$ is a 2×2 matrix. It turns out that the boundary form $[F_*, F_*](0)$ is determined by the first two terms on the right-hand side in representation (9.29) and essentially depends on the parameter Υ. Using the Cauchy–Schwarz inequality for estimating the integrals $I_1(r)$ and $I_2(r)$, we obtain (with logarithmic accuracy)

$$I_1(r) = O\left(r^{1/2}\right), I_2(r) = O\left(r^{1/2}\right), r \to 0. \tag{9.30}$$

Using the above estimates, we will fix the constants $c_{1,2}$ for different regions of the charge in what follows.

Finding the spectrum of operators $\hat{h}_{\mathfrak{e}}$, we follow the scheme that was described in Sect. 5.3.5 for a 2×2 matrix of differential operators.

In the case under consideration, any solution F of (5.34) allows the representation

$$\begin{aligned} F(r) &= c_1 F_1(r;W) + c_2 F_3(r;W) + \omega^{-1}(W) \\ &\times \left[\int_r^{\infty} [F_1(r;W) \otimes F_3(r';W)] \Psi(r') \mathrm{d}r' \right. \\ &\left. + \int_0^r F_3(r;W) \otimes F_1(r';W) \Psi(r') \mathrm{d}r' \right], \end{aligned} \tag{9.31}$$

where F_1, F_3, and ω are given by (9.16), (9.20), (9.21), and (9.22). This representation is well defined because $F_3(r;W)$ with $\operatorname{Im} W > 0$ decreases exponentially as $r \to \infty$. The condition $F \in \mathbb{L}^2(\mathbb{R}_+)$, which is sufficient for F to belong to $D_{h_{\mathfrak{e}}}$ (because then automatically $\check{h}F = WF + \eta \in \mathbb{L}^2(\mathbb{R}_+)$), implies $c_1 = 0$; otherwise, F is not square-integrable at infinity, since $F_1(r;W)$ with $\operatorname{Im} W > 0$ grows exponentially as $r \to \infty$. The constant c_2 is determined from the condition $F \in D_{h_{\mathfrak{e}}}$.

9.4.2 Nonsingular Region

In this nonsingular charge region, we have

$$0 < q \leq q_{\mathrm{s}}(j) \Longrightarrow \Upsilon_+ = \gamma \geq 1/2.$$

The representation (9.29) allows the evaluation of the asymptotic behavior of $F \in D^*_{\check{h}}(\mathbb{R}_+)$ at the origin. According to (9.28), the doublet $u_1(r) \sim r^{\gamma}$ is square-integrable at the origin, whereas the doublet $u_2(r) \sim r^{-\gamma}$ is not.

It follows that for $F_*(r)$ to belong to the space $\mathbb{L}^2(\mathbb{R}_+)$, it is necessary that the coefficient c_2 in front of $u_2(r)$ in (9.29) be zero; otherwise, F_* is not square-integrable at the origin (if $c_2 \neq 0$) because $F_3(r;W)$ is not square-integrable at the origin, which yields

$$F_*(r) = c_1 u_1(r) + I_1(r) + I_2(r) = O\left(r^{1/2}\right) \to 0,\ r \to 0,$$

whence it follows that for any $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$, we have

$$[F_*, F_*](0) = 0 \Longrightarrow \Delta_{h+}(F_*) = 0;$$

see (9.25) and the related discussion. This means that in the first noncritical charge region, the deficiency indices of the operator $\hat{h}$ are zero and the operator $\hat{h}_1 = \hat{h}^+$ is a unique s.a. extension of $\hat{h}$ with domain $D_{h_1} = D^*_{\check{h}}(\mathbb{R}_+)$.

We note that this result actually justifies the standard naïve treatment of the "Dirac Hamiltonian" with $q \leq \sqrt{3}/2$ ($Z \leq Z_{\mathrm{sc}} = \sqrt{3}/2\alpha \approx 119$) in the physics literature when the natural domain for $\check{h}$ is implicitly assumed.[11]

We thus obtain that the solution $F \in D_{h_1}$ of (5.34) is given by (9.31) with $c_1 = c_2 = 0$. Then, following Sect. 5.3.5, we obtain the Green's function of the operator $\hat{h}_1$,

$$G\left(r, r'; W\right) = \omega^{-1}(W) \begin{cases} F_3(r; W) \otimes F_1\left(r'; W\right), \ r > r', \\ F_1(r; W) \otimes F_3\left(r'; W\right), \ r < r'. \end{cases}$$

For the doublet U defining the guiding functional $\Phi(F; W)$ (5.33), we choose F_1. Such a guiding functional is simple, that is, satisfies the properties (i)–(iii) of Sect. 5.3.

Property (i) is evident, property (iii) is easily verified by integrating by parts, and it remains to verify property (ii): the equation $(\hat{h}_1 - E_0)\Psi(r) = F_0(r)$, where F_0 is in $\mathbb{D}$ and satisfies the condition $\Phi(F_0; E_0) = 0$, has a solution belonging to $\mathbb{D}$.

As such a solution, we choose a doublet

$$\Psi(r) = \int_r^\infty \left[F_1(r; E_0) \otimes F(y)\right] F_0(y) \mathrm{d}y + \int_0^r [F(r) \otimes F_1(y; E_0)] F_0(y) \mathrm{d}y, \tag{9.32}$$

where $F(r)$ is any solution of the equation $(\check{h} - E_0)F(r) = 0$ with the property $\mathrm{Wr}(F, F_1) = 1$. It is easy to prove that the function (9.32) belongs to $\mathbb{D}$.

In the region $l - 1 < 2\gamma < l + 1$, $l \in \mathbb{N}$, we represent F_3 in the form

$$\begin{aligned} \omega^{-1}(W) F_3 &= A_l(W) F_1 + q\,(2\gamma)^{-1} U_l, \\ U_l &= F_2 + a_l(W) \Gamma(-2\gamma) F_1, \\ A_l(W) &= \Gamma(-2\gamma) \left[\omega^{-1}(W) - \omega^{-1}(W)|_{\gamma = l/2}\right], \\ a_l(W) &= 2\gamma \left[q\omega(W)|_{\gamma = l/2}\right]^{-1}. \end{aligned} \tag{9.33}$$

[11] The uniqueness of the Hamiltonian also implies that the notion of δ potential for a relativistic Dirac particle cannot be introduced, which possibly manifests the nonrenormalizability of the four-fermion interaction.

The doublet U_l has a finite limit as $\gamma \to l/2$. A direct calculation (with the use of the equality $\Gamma(w+1) = w\Gamma(w)$) shows that $a_l(W)$ is a polynomial in W with real coefficients, and because F_1 and F_2 are real entire in W, the doublet U_l is also real entire.

Having the Green's function in hand, and using (9.33), we obtain

$$\begin{aligned} G(c-0, c+0; E+i0) &= \omega^{-1}(W) F_1(c;W) \otimes F_3(c;W) \\ &= A_l(W) F_1(c;W) \otimes F_1(c;W) + (q/2\gamma)\, F_1(c;W) \\ &\quad \otimes U_{(l)}(c;W). \end{aligned} \tag{9.34}$$

Due to the fact that $F_1(c;E)$ and $U_l(c;E)$ are real, it follows from (9.34) that $\sigma'(E) = \pi^{-1} \operatorname{Im} A_l(E+i0)$. Since the function $A_l(E+i\varepsilon)$ is continuous with respect to γ at the point $\gamma = l/2$, we can calculate $\sigma'(E)$ for $\gamma \neq l/2$ and then obtain it for $\gamma = l/2$:

$$\sigma'(E)|_{\gamma=l/2} = \lim_{\gamma \to l/2} \left[\sigma'(E)|_{\gamma \neq l/2} \right].$$

The expression $\sigma'(E)$ for $\gamma \neq l/2$ becomes rather simple:

$$\sigma'(E) = \pi^{-1} \Gamma(-2\gamma) \operatorname{Im} \omega^{-1}(E+i0).$$

At the points where the function $\omega(E+i0)$ is different from zero, we have $\sigma'(E) = \pi^{-1} \operatorname{Im} \omega^{-1}(E)$. For $|E| \geq m$ and

$$\Lambda = \sqrt{\frac{E-m}{E+m}},\ K = \epsilon k = \mathrm{e}^{(1-\epsilon)i\pi/2} k,\ k = \sqrt{E^2 - m^2} \geq 0,\ \epsilon = E/|E|,$$

a direct verification shows that $\omega(E)$ is continuous, $\omega(E) \neq 0$, and $\operatorname{Im} \omega(E) \neq 0$; the spectral function $\sigma(E)$ is a.c. and

$$\begin{aligned} \sigma'(E) &= \pi^{-1} \Gamma(-2\gamma) \operatorname{Im} \omega^{-1}(E), \\ \omega(E) &= \frac{\Gamma(1+2\gamma) \mathrm{e}^{\epsilon i \pi \gamma} \Gamma(-\gamma + q|E|/ik)[(\varkappa + \gamma)\epsilon k + iq(E-m)]}{q\Gamma(\gamma + q|E|/ik)[(\varkappa - \gamma)\epsilon k + iq(E-m)](2k/m)^{2\gamma}} \end{aligned}$$

(due to the properties of $\omega(E)$ described above, the limit of $\sigma'(E)$ as $2\gamma \to n \in \mathbb{N}$ exists). Thus, for $|E| \geq m$, the spectrum is continuous (and simple).

For $|E| < m$ and

$$\Lambda = i\sqrt{\frac{m-E}{m+E}},\ K = i\tau = \mathrm{e}^{i\pi/2}\tau,\ \tau = \sqrt{m^2 - E^2} > 0,$$

we have

$$\omega(E) = \frac{\Gamma(1+2\gamma)\Gamma\left(-\gamma - qE\tau^{-1}\right)[q(m-E) - (\varkappa + \gamma)\tau]}{q\Gamma(\gamma - qE/\tau)[q(m-E) - (\varkappa - \gamma)\tau](2\tau/m)^{2\gamma}}.$$

We stress that $\omega(E)$ is real, and $\operatorname{Im}\omega^{-1}(E+i0)$ can differ from zero only at the points where $\omega(E)=0$. Since $\Gamma(x)$ does not vanish for real x, the function $\omega(E)$ can vanish only at the points where E satisfies one of the following two conditions:

Condition (a):

$$q(m-E)-(\varkappa+\gamma)\tau=0.$$

Condition (b):

$$\gamma-qE\tau^{-1}=-n\in\mathbb{Z}_+.$$

In case (a), solutions for E do not exist if $\zeta=-1$. For $\zeta=1$, we have $E=-\gamma m\varkappa^{-1}$. At this point, $\gamma+qE\tau^{-1}=0$, so that

$$\Gamma\left(-\gamma-qE\tau^{-1}\right)[q(m-E)-(\varkappa+\gamma)\tau]\neq 0,\ \omega(E)\neq 0.$$

In case (b), which defines the points where $\Gamma\left(\gamma-qE\tau^{-1}\right)=\infty$, there exist solutions $\overset{I}{E}_n$,

$$\overset{I}{E}_n=m\,(n+\gamma)\left[q^2+(n+\gamma)^2\right]^{-1/2},$$
$$\tau_n=qm\left[q^2+(n+\gamma)^2\right]^{-1/2},\ n\in\mathbb{Z}_+.$$

But for $\zeta=1$ at the point $E=\overset{I}{E}_0$, we also have $q(m-\overset{I}{E}_0)-(\varkappa-\gamma)\tau_0=0$, and consequently,

$$\left|\Gamma\left(\gamma-q\overset{I}{E}_0\tau_0^{-1}\right)\left[q\left(m-\overset{I}{E}_0\right)-(\varkappa-\gamma)\tau_0\right]\right|<\infty.$$

We thus obtain that $\omega(E)$ vanishes at the discrete points $\overset{I}{E}_n$,

$$\overset{I}{E}_n=m\,(n+\gamma)\left[q^2+(n+\gamma)^2\right]^{-1/2},$$
$$n\in\mathcal{N}_\zeta,\ \mathcal{N}_\zeta=\begin{cases}\mathbb{N},\ \zeta=1,\\ \mathbb{Z}_+,\ \zeta=-1,\end{cases} \tag{9.35}$$

which form the well-known discrete spectrum of bound states of the Dirac electron in the Coulomb field with $Z<Z_{\mathrm{c}}$.

We note that the discrete spectrum is accumulated at the point $E=m$, and its asymptotic form as $n\to\infty$ reads

$$E_n^{\mathrm{nonrel}}\equiv m-E_n=mq^2\left(2n^2\right)^{-1}, \tag{9.36}$$

which is the well-known nonrelativistic formula for bound-state energies of an electron in a Coulomb field.

In a neighborhood of the points $\overset{I}{E}_n$, we have

$$\Gamma(-2\gamma)\omega^{-1}(E+i0) = -Q_n^2\left(E-\overset{I}{E}_n+i0\right)^{-1} + O(1),$$

$$Q_n^2 = \Gamma(-2\gamma)\left[\omega'(\overset{I}{E}_n)\right]^{-1},$$

$$Q_n = \sqrt{\frac{\Gamma(2\gamma+1+n)\tau_n^3(2\tau_n/m)^{2\gamma}\left[q\left(m-\overset{I}{E}_n\right)-(\varkappa-\gamma)\tau_n\right]}{m^2 n!\Gamma^2(2\gamma+1)\left[q\left(m-\overset{I}{E}_n\right)-(\varkappa+\gamma)\tau_n\right]}}.$$

It is easy to check that $\operatorname{Im} O(1) = 0$ and obviously that Q_n^2 is positive, which is in agreement with predictions of the general theory.

It follows that for $|E| < m$, the spectral function $\sigma(E)$ is a jump function with jumps Q_n^2 located at the points $E = \overset{I}{E}_n > 0$, and

$$\sigma'(E) = \sum_{n\in\mathcal{N}_\zeta} Q_n^2\delta\left(E-\overset{I}{E}_n\right),\ |E| < m.$$

Thus, the simple spectrum of $\hat{h}_1$ is given by

$$\operatorname{spec}\hat{h}_1 = \{|E| \geq m\} \cup \left\{\overset{I}{E}_n,\ n\in\mathcal{N}_\zeta\right\}.$$

The generalized eigenvectors $U_E(r)$, $|E| \geq m$, and eigenvectors $U_n(r)$ of $\hat{h}_1$,

$$\begin{aligned} U_E(r) &= \overset{I}{U}_E(r) = \sqrt{\sigma'(E)}F_1(r;E),\ |E| \geq m; \\ U_n(r) &= \overset{I}{U}_n(r) = Q_n F_1\left(r;\overset{I}{E}_n\right),\ n\in\mathcal{N}_\zeta, \end{aligned} \tag{9.37}$$

form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$.

9.4.3 Singular Region

In the singular regions, $Z > Z_s(j)$, the deficiency indices of the operators $\hat{h}$ are $(1,1)$, and therefore, there exists a family $\{\hat{h}_\nu\}$ of s.a. extensions of $\hat{h}$ parameterized by a parameter $\nu \in [-\pi/2, \pi/2]$, $-\pi/2 \sim \pi/2$. Technically, it is convenient to divide the singular region into three subregions, which we call the subcritical, critical, and overcritical regions. The subregions are distinguished by a character of asymptotic boundary conditions at the origin specifying the domains D_{h_ν} of the operators $\hat{h}_\nu$ and providing their self-adjointness. The boundary conditions are similar in each subregion, which provides similar solutions of the corresponding spectral problems. In what follows, we describe these subregions, the domains D_{h_ν} in these subregions, and details of discrete spectra.

9.4.4 Subcritical Region

In this subcritical charge region, we have

$$q_s(j) < q < q_c(j) \Longrightarrow 0 < \Upsilon_+ = \gamma < 1/2.$$

Here we evaluate the asymptotic behavior of doublets $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$ at the origin with the use of the representation (9.29). In the case under consideration, both $u_1(r) \sim r^\gamma$ and $u_2(r) \sim r^{-\gamma}$ are square-integrable at the origin and estimates (9.30) hold, so that for any $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$, we have

$$F_*(r) = c_1(mr)^\gamma d_+ + c_2(mr)^{-\gamma} d_- + O\left(r^{1/2}\right), r \to 0,$$

which in turn yields

$$\Delta_{h^+}(F_*) = 2\gamma q^{-1} \left(\overline{c_2}\, c_1 - \overline{c_1}\, c_2\right), \tag{9.38}$$

with account taken of (9.26) and (9.25). The expression (9.38) for the asymmetry form $\Delta_{h^+}(F_*)$ implies that the deficiency indices of $\hat{h}$ are $m_\pm = 1$, and therefore there exists a family of s.a. extensions $\hat{h}_{2,\nu}$ of $\hat{h}$ parameterized by[12] $\nu \in \mathbb{S}(-\pi/2, \pi/2)$, with domains $D_{h_{2,\nu}}$, specified by s.a. boundary conditions

$$F(r) = c\left[(mr)^\gamma d_+ \cos\nu + (mr)^{-\gamma} d_- \sin\nu\right] + O\left(r^{1/2}\right), r \to 0 \tag{9.39}$$

(c is an arbitrary complex number) and having the form

$$D_{h_\nu} = \left\{F(r) : F(r) \in D^*_{\check{h}}(\mathbb{R}_+),\ F \text{ obey } (9.39)\right\}.$$

[12] It should be borne in mind that the extension parameters depend on both j and ζ. The same remark holds for all the subsequent regions.

The spectral analysis in this charge region is quite similar to that in the first noncritical region. We therefore only point out necessary modifications and formulate final results.

For the doublet U defining guiding functional $\Phi(F, W)$ (5.33), we choose the solution $U_\nu = F_1 \cos\nu + F_2 \sin\nu$, where F_1 and F_2 are given by formulas (9.16)–(9.18). The solution U_ν is real entire in W and satisfies the asymptotic condition (9.39). The guiding functional with the chosen U_ν is simple.

The Green's function of the s.a. operator $\hat{h}_{2,\nu}$ has the form

$$G\left(r, r'; W\right) = \omega_1^{-1}(W) \begin{cases} F_3(r; W) \otimes U_\nu\left(r'; W\right), r > r', \\ U_\nu(r; W) \otimes F_3\left(r'; W\right), r < r', \end{cases}$$
$$\omega_1(W) = -\operatorname{Wr}(F_1, F_3) = \omega(W)\cos\nu + q^{-1}\Gamma(1-2\gamma)\sin\nu. \tag{9.40}$$

Using the relations

$$F_3 = q\,(2\gamma)^{-1}\left[\tilde{\omega}_1 U_\nu + \omega_1 \tilde{U}_\nu\right],$$
$$\tilde{U}_\nu = \tilde{U}_\nu(r; W) = -F_1(r; W)\sin\nu + F_2(r; W)\cos\nu,$$
$$\tilde{\omega}_1 = \tilde{\omega}_1(W) = \omega(W)\sin\nu - q^{-1}\Gamma(1-2\gamma)\cos\nu,$$

and (9.40), we obtain

$$G(c-0, c+0; E+i0) = \omega_2^{-1}(W) U_\nu(c; W) \otimes U_\nu(c; W)$$
$$+ q\,(2\gamma)^{-1}\,\tilde{U}_\nu(c; W) \otimes U_\nu(c; W),$$
$$\omega_2(W) = 2\gamma\omega_1(W)[q\tilde{\omega}_1(W)]^{-1}.$$

Since both $U_\nu(c; E)$ and $\tilde{U}_\nu(c; E)$ are real, the derivative $\sigma'(E)$ of the spectral function is given by $\sigma'(E) = \pi^{-1}\operatorname{Im}\omega_2^{-1}(E+i0)$.

At the points where the function $\omega_2(E)$ is different from zero, we have $\omega_2^{-1}(E+i0) = \omega_2^{-1}(E)$.

For $E \geq m$ and $E < -m$, the function $\omega_2(E)$ is continuous, $\omega_2(E) \neq 0$, and $\sigma'(E) = \pi^{-1}\operatorname{Im}\omega_2^{-1}(E) \neq 0$. The spectral function $\sigma(E)$ is therefore a.c. Thus, the spectrum is continuous and simple (the continuous spectrum includes the point $E = -m$ as well). However, in the case $E = -m$, we have

$$\sigma'(-m)\big|_{\nu=\nu_{-m}} = \infty, \ \tan\nu_{-m} = -(2q)^{-2\gamma}\Gamma^{-1}(1-2\gamma)\Gamma(1+2\gamma).$$

The range $\nu \sim \nu_{-m}$, $E \sim -m$ requires more detailed consideration. Here we obtain

$$\begin{aligned}
\sigma'(E) &= \pi^{-1}\,\mathrm{Im}\,\tilde{\omega}_2^{-1}(E+i0) + O(1),\\
\tilde{\omega}_2(W) &= 2\gamma q^{-1}\\
&\quad\times(\tan\nu_{-m} - \tan\nu)\cos^2\nu - \Psi^{-2}\Delta\cos^2\nu + O\left(\Delta^2\right),\\
\Delta &= W + m, W \to -m,\\
\Psi &= \frac{q(2q)^{\gamma}}{2\gamma}\sqrt{\frac{qm\Gamma(1-2\gamma)}{(q_{\mathrm{c}}^2 - \zeta q_{\mathrm{c}}/2 - 2\gamma^2/3)\Gamma(2+2\gamma)}}.
\end{aligned}$$

One can see that for $\nu \neq \nu_{-m}$, the function $\sigma'(E)$ is finite as $E \to -m$. However, at $\nu = \nu_{-m}$ and for small $E + m$, we have

$$\begin{aligned}
\sigma'(E) &= -\frac{\Psi^2\cos^{-2}\nu_{-m}}{\pi}\,\mathrm{Im}\,(E+m+i0)^{-1} + O(1)\\
&= \frac{\Psi^2}{\cos^2\nu_{-m}}\delta(E+m) + O(1),
\end{aligned}$$

that is, there is an eigenvalue $E = -m$ in the spectrum of $\hat{h}_{2,\nu_{-m}}$.

For $|E| < m$, the function $\omega(E)$ is real, and therefore, the function $\omega_2(E)$ is also real. As in the case of the nonsingular region, Sect. 9.4.2, it follows that for $|E| < m$, the spectral function $\sigma(E)$ is a jump function with the jumps $Q_n^2 = -[\omega_2'(\overset{II}{E}_n)]^{-1}, \omega_2'(\overset{II}{E}_n) < 0$, located at the points $\overset{II}{E}_n$ that satisfy the equation

$$\omega_2\left(\overset{II}{E}_n\right) = 0, \overset{II}{E}_n = \overset{II}{E}_n(\nu)\,. \tag{9.41}$$

As a result, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta\left(E - \overset{II}{E}_n\right), |E| < m.$$

We note that as in the first noncritical charge region, there are infinitely many energy levels accumulated at the point $E = m$, and their asymptotic form as $n \to \infty$ is given by the nonrelativistic expression (9.36), which does not depend on ν. The lower bound state energy essentially depends on ν, and there exists a value of $\nu = \nu_{-m}$ for which the lower bound state energy coincides with the boundary $E = -m$ of the lower (positron) continuous spectrum. Some results relating to numerical solution of equation (9.41) are presented in Fig. 9.1.

Thus, the simple spectrum of $\hat{h}_{2,\nu}$ is given by spec $\hat{h}_{2,\nu} = \{|E| \geq m\} \cup \{\overset{II}{E}_n\}$.

The generalized eigenvectors $U_E(r)$, $|E| \geq m$, and eigenvectors $U_n(r)$ of $\hat{h}_{2,\nu}$,

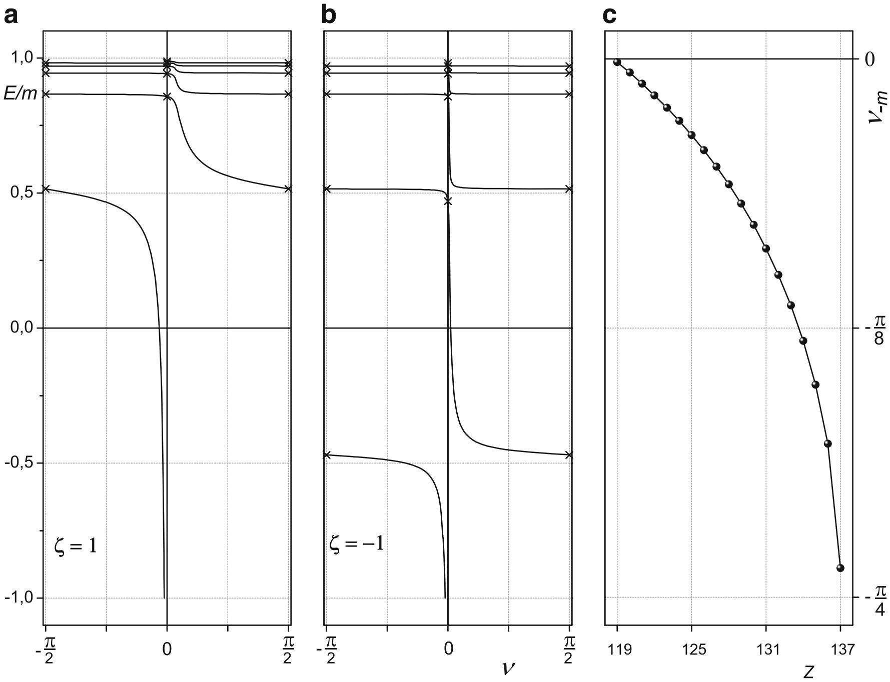

Fig. 9.1 ν-dependence of energy levels $\overset{II}{E}_n$ for $Z = 121$, $j = 1/2, \zeta = \pm 1$, and Z-dependence of ν_{-m}, $j = 1/2$

$$
\begin{aligned}
U_E(r) &= \overset{II}{U}{}_E^{\nu}(r) = \sqrt{\sigma'(E)}U_\nu(r;E), \ |E| \geq m; \\
U_n(r) &= \overset{II}{U}{}_n^{\nu}(r) = Q_n U_\nu\left(r; \overset{II}{E}_n\right),
\end{aligned}
\tag{9.42}
$$

form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$.

It is possible to describe the discrete spectrum in more detail. Explicit expressions for the spectrum and eigenfunctions can be obtained in two cases. For $\nu = \pi/2$, we have

$$
\omega_2(W) = 2\gamma\Gamma(1-2\gamma)\left[q^2\omega(W)\right]^{-1}, U_{\nu=\pi/2}(r;W) = F_2(r;W).
$$

The corresponding analysis is identical to that in Sect. 9.4.2, and all the results (for the spectrum and eigenfunctions) can be obtained from the corresponding expressions of the previous subsection with the help of the formal substitution $\gamma \to -\gamma$. In particular, we obtain that the discrete spectrum $\overset{II}{\mathcal{E}}_n$ of $\hat{h}_{2,\pm\pi/2}$ has the form

$$
\overset{II}{\mathcal{E}}_n = \frac{(n-\gamma)m}{\sqrt{q^2 + (n-\gamma)^2}}, \ n \in \mathcal{N}_\zeta.
$$

For $\nu = 0$, we have

$$\omega_2(W) = \omega(W)\Gamma^{-1}(-2\gamma),\ U_{\nu=0}(r;W) = F_1(r;W),$$

so that the corresponding analysis is identical to that in Sect. 9.4.2, and the expressions obtained there directly serve for the region $0 < \gamma < 1/2$. In particular, we obtain that the discrete spectrum $\overset{II}{E}_n(0)$ of $\hat{h}_{2,0}$ is given by (9.35).

For $|\nu| < \pi/2$, the equation $\omega_2(\overset{II}{E}_n) = 0$ can be represented in the equivalent form

$$\begin{aligned}
\omega\left(\overset{II}{E}_n\right) &= -q^{-1}\Gamma(1-2\gamma)\tan\nu,\\
\omega'\left(\overset{II}{E}_n\right) &= -\frac{\Gamma(1-2\gamma)}{2\gamma\cos^2\nu}\omega_2'\left(\overset{II}{E}_n\right) > 0,\\
\partial_\nu \overset{II}{E}_n &= -\frac{\Gamma(1-2\gamma)}{q\omega'\left(\overset{II}{E}_n(\nu)\right)\cos^2\nu} < 0.
\end{aligned} \tag{9.43}$$

The function $\omega(E)$ has the properties

$$\begin{aligned}
&\omega(-m) = q^{-1}\Gamma(1+2\gamma)(2q)^{-2\gamma} + 0;\\
&\omega\left(\overset{II}{\mathcal{E}}_n \pm 0\right) = \mp\infty;\ \omega\left(\overset{II}{E}_n(0)\right) = 0,\\
&\overset{II}{\mathcal{E}}_n < \overset{II}{E}_n(0) < \overset{II}{\mathcal{E}}_{n+1},\ n \geq n_\zeta,\ n_1 = 1,\ n_{-1} = 0,\ \overset{II}{\mathcal{E}}_{n_\zeta} > -m.
\end{aligned}$$

It follows from these properties that there are no spectrum points in the interval $[-m, \overset{II}{\mathcal{E}}_{n_\zeta})$ for $\nu \in (\nu_{-m}, \pi/2)$, and for fixed $\nu \in [\nu_{-m}, -\pi/2)$, there is one level $\overset{II}{E}_{n_\zeta - 1}(\nu)$ monotonically growing from $-m$ to $\overset{II}{\mathcal{E}}_{n_\zeta} - 0$ as ν goes from ν_{-m} to $-\pi/2 + 0$; in each interval $(\overset{II}{\mathcal{E}}_n, \overset{II}{\mathcal{E}}_{n+1})$, for a fixed $\nu \in (-\pi/2, \pi/2)$, there is one level $\overset{II}{E}_n(\nu)$ monotonically growing from $\overset{II}{\mathcal{E}}_n + 0$ to $\overset{II}{\mathcal{E}}_{n+1} - 0$ as ν goes from $\pi/2 - 0$ to $-\pi/2 + 0$. Note the relationships

$$\lim_{\nu\to-\pi/2} \overset{II}{E}_{n-1}(\nu) = \lim_{\nu\to\pi/2} \overset{II}{E}_n(\nu) = \overset{II}{\mathcal{E}}_n,\ n \in \mathcal{N}_\zeta.$$

9.4.5 Critical Region

The critical region is the critical curve $Z = Z_c(j)$. In this critical charge region, we have

$$q = q_c(j) \Longrightarrow \Upsilon_+ = \gamma = 0.$$

The charge values $q = q_c(j)$ stand out because for $q > q_c(j)$, the standard formula (9.35) for the bound-state spectrum ceased to be true, yielding complex energy values. But we will see that from a mathematical standpoint, nothing extraordinary happens with the system for the charge values $q \geq q_c(j)$, at least in comparison with the previous case of $q_s(j) < q < q_c(j)$.

It should also be noted that this region does not exist if the finite structure constant α is an irrational number, because here the relation $\alpha = (j + 1/2)/Z$ must hold.

It follows from representations (9.23) and (9.24) that the asymptotic behavior of doublets $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$ in the case under consideration is given by

$$F_*(r) = c_1 d_+ + c_2 d_0(r) + O\left(r^{1/2}\ln r\right), r \to 0,$$

which yields the expression $\Delta_{h^+}(F_*) = q_c^{-1}(j)\left(\overline{c_1}c_2 - \overline{c_2}c_1\right)$ for the asymmetry form. Therefore, here, we also have a one-parameter $U(1)$ family of s.a. extensions $\hat{h}_{3,\vartheta}$, $\vartheta \in \mathbb{S}(-\pi/2, \pi/2)$, specified by s.a. asymptotic boundary conditions

$$F(r) = c\left[d_0(r)\cos\vartheta + d_+ \sin\vartheta\right] + O\left(r^{1/2}\ln r\right), r \to 0, \tag{9.44}$$

and the corresponding domains $D_{h_{3,\vartheta}}$ are

$$D_{h_{3,\vartheta}} = \left\{F(r) : F \in D^*_{\check{h}}(\mathbb{R}_+), F \text{ obey } (9.44)\right\}.$$

The spectral analysis follows in the standard way presented in the previous subsections, and therefore, we only cite the final results. For the doublet U defining the guiding functional (5.33), we choose the doublet $U^{(0)}_\vartheta = F^{(0)}_1 \sin\vartheta + F^{(0)}_2 \cos\vartheta$, real entire in W, where $F^{(0)}_1$ and $F^{(0)}_2$ are given by (9.23). The doublet $U^{(0)}_\vartheta$ satisfies the s.a. asymptotic boundary conditions (9.44). The guiding functional with this $U^{(0)}_\vartheta$ is simple.

The Green's function $G(r, r'; W)$ of the Hamiltonian $\hat{h}_{3,\vartheta}$ is given by

$$G(r, r'; W) = \omega_3^{-1}(W)\begin{cases} F^{(0)}_3(r; W) \otimes U^{(0)}_\vartheta(r'; W), & r > r', \\ U^{(0)}_\vartheta(r; W) \otimes F^{(0)}_3(r'; W), & r < r', \end{cases}$$

$$F^{(0)}_3 = q_c(j)\,\tilde{\omega}_3(W)U^{(0)}_\vartheta + q_c(j)\,\tilde{U}^{(0)}_\vartheta,$$

$$\tilde{U}_{\vartheta}^{(0)} = F_1^{(0)} \cos\vartheta - F_2^{(0)} \sin\vartheta,$$
$$\omega_3(W) = -\mathrm{Wr}\left(U_{\vartheta}^{(0)}, F_3^{(0)}\right) = q_{\mathrm{c}}^{-1}(j)\,[f(W)\cos\vartheta - \sin\vartheta],$$
$$\tilde{\omega}_3(W) = q_{\mathrm{c}}^{-1}(j)\,[f(W)\sin\vartheta + \cos\vartheta].$$

The derivative $\sigma'(E)$ of the spectral function reads

$$\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\omega_4^{-1}(E+i0), \omega_4(W) = [q_{\mathrm{c}}(j)\,\tilde{\omega}_3(W)]^{-1}\,\omega_3(W).$$

At the points where the function $\omega_4(E)$ is different from zero, we have $\omega_4^{-1}(E+i0) = \omega_4^{-1}(E)$.

For $|E| \geq m$ and $K = \epsilon k = \mathrm{e}^{(1-\epsilon)i\pi/2}k, k = \sqrt{E^2-m^2} \geq 0, \epsilon = |E|/E$, the function $f(E)$ is given by

$$f(E) = \ln[2\mathrm{e}^{-i\epsilon\pi/2}km^{-1}] + \psi\left(-iq_{\mathrm{c}}(j)\,|E|k^{-1}\right)$$
$$+ \frac{\left[\zeta + (i\epsilon k - \zeta m)\,E^{-1}\right]}{2q_{\mathrm{c}}(j)} - 2\psi(1).$$

In the regions $E \geq m$ and $E < -m$, $K = \epsilon k = \mathrm{e}^{i\pi}k$, the function $\omega_4(E)$ is continuous, different from zero, complex, and $\sigma'(E) = \pi^{-1}\,\mathrm{Im}\,\omega_3^{-1}(E) \neq 0$. Therefore the spectral function $\sigma(E)$ is a.c., and the spectrum is continuous and simple (the continuous spectrum includes also the point $E = -m$). However, in the case $E = -m$, we have $\sigma'(-m)|_{\vartheta=\vartheta_{-m}} = \infty$, where

$$\tan\vartheta_{-m} = \ln(2q_{\mathrm{c}}) - 2\psi(1) + \zeta/q_{\mathrm{c}} = \ln(2q_{\mathrm{c}}) + (2\mathbf{C} + \zeta/q_{\mathrm{c}}) > 0,$$

and therefore the range $\vartheta \sim \vartheta_{-m}$, $E \sim -m$ requires a more detailed consideration. Here we obtain

$$\sigma'(E) = \frac{q_{\mathrm{c}}}{\pi\cos^2\vartheta}\,\mathrm{Im}\,\tilde{\omega}_4^{-1}(E+i0) + O(1),\ \tilde{\omega}_4(W) = (\tan\vartheta_{-m} - \tan\vartheta)$$
$$- \Psi^{-2}\Delta + O(\Delta^2),\ \Delta = W + m,\ \Psi = \sqrt{\frac{q_{\mathrm{c}}m}{1-\zeta/2q_{\mathrm{c}}}},\ W \to -m.$$

One can see that for $\vartheta \neq \vartheta_{-m}$, the function $\sigma'(E)$ is finite as $E \to -m$. However, at $\vartheta = \vartheta_{-m}$ and for small $E+m$, we have

$$\sigma'(E) = -\frac{\Psi^2}{\pi\cos^2\vartheta_{-m}}\,\mathrm{Im}\,(E+m+i0)^{-1} + O(1)$$
$$= \frac{\Psi^2}{\cos^2\vartheta_{-m}}\delta(E+m) + O(1),$$

that is, there is an eigenvalue $E = -m$ in the spectrum of $\hat{h}_{3,\vartheta_{-m}}$.

For $|E| < m$ and $K = i\tau = e^{i\pi/2}\tau$, $\tau = \sqrt{m^2 - E^2} > 0$, the function $f(E)$ is given by

$$f(E) = \ln\left(2\tau m^{-1}\right) + \psi\left(-q_c(j)\, E\tau^{-1}\right) + \frac{\zeta - (\tau + \zeta m)\, E^{-1}}{2q_c(j)} + 2\mathbf{C}. \quad (9.45)$$

It is real, and therefore the function $\omega_4(E)$ is also real.

As in the previous cases, the spectral function $\sigma(E)$ for $|E| < m$ is a jump function with the jumps $Q_n^2 = -[\omega_4'(\overset{III}{E_n})]^{-1}$ located at the discrete energy levels $\overset{III}{E_n}$ determined by the equations

$$\omega_4\left(\overset{III}{E_n}\right) = 0,\ \omega_4'\left(\overset{III}{E_n}\right) < 0,\ \overset{III}{E_n} = \overset{III}{E_n}(\vartheta), \quad (9.46)$$

so that

$$\sigma'(E) = \sum_n Q_n^2 \delta\left(E - \overset{III}{E_n}\right).$$

We note that there exists an infinite number of discrete levels, which are accumulated at the point $E = m$, and their asymptotic behavior as $n \to \infty$ is described by the nonrelativistic formula (9.36).

The lower bound state of energy essentially depends on ϑ, and there exists such a value of $\vartheta = \vartheta_{-m}$ for which the lower bound state energy coincides with the boundary $E = -m$ of the lower (positron) continuous spectrum.

Thus, the simple spectrum of $\hat{h}_{3,\vartheta}$ is given by spec $\hat{h}_{3,\vartheta} = \{|E| \geq m\} \cup \{\overset{III}{E_n}\}$. The generalized eigenvectors $U_E(r)$, $|E| \geq m$, and eigenvectors $U_n(r)$ of $\hat{h}_{3,\vartheta}$,

$$\begin{aligned} U_E(r) &= \overset{III}{U_E^{\vartheta}}(r) = \sqrt{\sigma'(E)}U_{\vartheta}^{(0)}(r; E),\ \ |E| \geq m; \\ U_n(r) &= \overset{III}{U_n^{\vartheta}}(r) = Q_n U_{\vartheta}^{(0)}\left(r; \overset{III}{E_n}\right), \end{aligned} \quad (9.47)$$

form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$.

For $\vartheta = \pi/2$, it is possible to obtain the explicit formulas for spectrum and eigenvectors of a complete set. Here,

$$\omega_4(W) = -\left[q_c(j)\, f(W)\right]^{-1},\ U_{\vartheta=\pi/2}^{(0)} = F_1^{(0)},$$

and

$$\sigma'(E) = -\pi^{-1} q_c(j)\, \mathrm{Im}\, f(E + i0).$$

For $|E| \geq m$ and $K = \epsilon k = \mathrm{e}^{(1-\epsilon)i\pi/2}k$, $k = \sqrt{E^2 - m^2} \geq 0$, $\epsilon = E/|E|$, we have

$$\sigma'(E) = [q_c(j)/2]\,[\coth(q_c(j)\,|E|/k) + \epsilon]\,.$$

The spectrum is simple and continuous.

For $|E| < m$, and $K = i\tau = \mathrm{e}^{i\pi/2}\tau$, $\tau = \sqrt{m^2 - E^2} > 0$, we obtain

$$\sigma'(E) = \sum_{n \in \mathcal{N}_\zeta} Q_n^2 \delta\left(E - \overset{III}{\mathcal{E}_n}\right),\; Q_n = \tau_n^{3/2}/m,$$
$$\overset{III}{\mathcal{E}_n} = mn(q_c^2 + n^2)^{-1/2},\; \tau_n = q_c m(q_c^2 + n^2)^{-1/2},\; n \in \mathcal{N}_\zeta.$$

Thus, the simple spectrum of $\hat{h}_{3,\pi/2}$ is given by spec $\hat{h}_{3,\pi/2} = \{|E| \geq m\} \cup \{\overset{III}{\mathcal{E}_n}\}$. The generalized eigenvectors $U_E(r)$, $|E| \geq m$, and eigenvectors $U_n(r)$ of $\hat{h}_{3,\pi/2}$,

$$U_E(r) = \overset{III}{U_E^{\pi/2}} = \sqrt{\sigma'(E)}U^{(0)}_{\vartheta=\pi/2}(r; E),\; |E| \geq m;$$
$$U_n(r) = \overset{III}{U_E^{\pi/2}} = Q_n U^{(0)}_{\vartheta=\pi/2}\left(r; \overset{III}{\mathcal{E}_n}\right),\; n \in \mathcal{N}_\zeta,$$

form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$.

We note that all the above results for the spectrum and for the inversion formulas can be obtained from the corresponding expressions of the first charge region in the limit $\gamma \to 0$.

For $|\vartheta| < \pi/2$, it is also possible to describe the discrete spectrum in more detail. In this case, (9.46) can be represented in the equivalent form

$$f\left(\overset{III}{E_n}\right) = \tan\vartheta,\; f'\left(\overset{III}{E_n}\right) = \frac{q_c}{\cos^2\vartheta}\omega_4'\left(\overset{III}{E_n}\right) < 0,$$
$$\partial_\vartheta \overset{III}{E_n} = \left[f'\left(\overset{III}{E_n}\right)\cos^2\vartheta\right]^{-1} < 0, \tag{9.48}$$

where the function $f(E)$ is given by (9.45) and has the properties

$$f(-m) = \ln(2q_c) + (2\mathbf{C} + \zeta/q_c) - 0;\; f\left(\overset{III}{\mathcal{E}_n} \pm 0\right) = \pm\infty;$$
$$\overset{III}{\mathcal{E}_n} < \overset{III}{\mathcal{E}_{n+1}},\; n \geq n_\zeta,\; n_1 = 1,\; n_{-1} = 0,\; \overset{III}{\mathcal{E}_{n_\zeta}} > -m.$$

Thus, we come to the following conclusion: there are no spectrum points in the interval $[-m, \overset{III}{\mathcal{E}}_{n_\zeta})$ for $\vartheta \in (\vartheta_{-m}, \pi/2)$, and for $\vartheta \in (-\pi/2, \vartheta_{-m}]$, there is one level $\overset{III}{E}_{n_\zeta - 1}(\vartheta)$ monotonically growing from $-m$ to $\overset{III}{\mathcal{E}}_{n_\zeta} - 0$ as ϑ goes from ϑ_{-m} to $-\pi/2 + 0$; in each interval $(\overset{III}{\mathcal{E}}_n, \overset{III}{\mathcal{E}}_{n+1})$, for $\vartheta \in (-\pi/2, \pi/2)$, there is one level $\overset{III}{E}_n(\vartheta)$ monotonically growing from $\overset{III}{\mathcal{E}}_n + 0$ to $\overset{III}{\mathcal{E}}_{n+1} - 0$ as ϑ goes from $\pi/2 - 0$ to $-\pi/2 + 0$.

9.4.6 Overcritical Region

In this overcritical charge region, we have $Z > Z_c(j)$ and

$$q > q_c(j) \Longrightarrow \Upsilon_+ = i\sigma,\ \sigma = \sqrt{q^2 - \varkappa^2} > 0.$$

According to representation (9.29), the asymptotic behavior of doublets $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$ in the case under consideration is given by

$$F_*(r) = c_1(mr)^{i\sigma} d_+ + c_2(mr)^{-i\sigma} d_- + O\left(r^{1/2}\right), r \to 0, \forall F_* \in D^*_{\check{h}}(\mathbb{R}_+),$$

where $d_\pm = \left(1 \big/ (\varkappa \pm i\sigma)\, q^{-1}\right)$, which yields $\Delta_{h+}(F_*) = 2i\sigma q^{-1}\left(|c_1|^2 - |c_2|^2\right)$ for the asymmetry form. It follows that we have a one-parameter $U(1)$ family of s.a. extensions $\hat{h}_{4,\theta}, \theta \in \mathbb{S}(0,\pi)$, specified by s.a. asymptotic boundary conditions

$$F(r) = c\left[e^{i\theta}(mr)^{i\sigma} d_+ + e^{-i\theta}(mr)^{-i\sigma} d_-\right] + O\left(r^{1/2}\right), r \to 0, \tag{9.49}$$

and acting on the domains $D_{h_{4,\theta}}$,

$$D_{h_{4,\theta}} = \left\{F(r) : F(r) \in D^*_{\check{h}}(\mathbb{R}_+),\ F \text{ obey } (9.49)\right\}.$$

For the doublet U defining the guiding functional (5.33), we choose $U_\theta = e^{i\theta}F_1 + e^{-i\theta}F_2$, where F_1 and F_2 are given by (9.16)–(9.18); U_θ is real entire in W because $F_2 = \overline{F_1}$ for $\Upsilon_+ = i\sigma$ and satisfies the boundary condition (9.49). Then one can verify that the guiding functional is simple.

The Green's function of the Hamiltonian $\hat{h}_{4,\theta}$ has the form

$$\begin{aligned} G(r, r'; W) &= \omega_6^{-1}(W) U_\theta(r; W) \otimes U_\theta(r'; W) \\ &\quad - \frac{2}{4\sigma}\begin{cases} \tilde{U}_\theta(r; W) \otimes U_\theta(r'; W),\ r > r', \\ U_\theta(r; W) \otimes \tilde{U}_\theta(r'; W),\ r < r', \end{cases} \end{aligned}$$

where

$$\begin{aligned}
\tilde{U}_\theta &= i\left[\mathrm{e}^{-i\theta}F_2 - \mathrm{e}^{i\theta}F_1\right],\\
2F_3 &= \Gamma(-2i\sigma)\mathrm{e}^{-i\theta}\left\{\left[1+\mathrm{e}^{2i\theta}\omega_5(W)\right]U_\theta + i\left[1-\mathrm{e}^{2i\theta}\omega_5\right]\tilde{U}_\theta\right\},\\
\omega_5(W) &= -q\omega(W)/\Gamma(1-2i\sigma),\ \omega_6(W) = -4i\sigma q^{-1}\frac{1-\omega_5(W)\mathrm{e}^{2i\theta}}{1+\omega_5(W)\mathrm{e}^{2i\theta}}.
\end{aligned}$$

The derivative of the spectral function is $\sigma'(E) = \pi^{-1}\operatorname{Im}\omega_6^{-1}(E+i0)$. At the points where the function $\omega_6(E+i0)$ is different from zero, we have $\omega_6^{-1}(E+i0) = \omega_6^{-1}(E)$.

For $E \geq m$ and $E < -m$, $K = \epsilon k = \mathrm{e}^{i(1-\epsilon)\pi/2}k$, $k = \sqrt{E^2-m^2} \geq 0$, $\epsilon = E/|E|$, the function $\omega_6(E)$ is continuous, complex, and differs from zero. Therefore $\sigma'(E) = \pi^{-1}\operatorname{Im}\omega_6^{-1}(E) \neq 0$, the spectral function $\sigma(E)$ is a.c., so that the spectrum is continuous and simple (the continuous spectrum includes the point $E = -m$ as well). However, for $E = -m$, we have

$$\sigma'(-m)\big|_{\theta=\theta_{-m}} = \infty,\ \mathrm{e}^{2i\theta_{-m}} = (2q)^{2i\sigma}\Gamma(-2i\sigma)\Gamma^{-1}(2i\sigma), \tag{9.50}$$

and therefore the range $\theta \sim \theta_{-m}$, $E \sim -m$ requires a more detailed consideration. Here we obtain

$$\begin{aligned}
\sigma'(E) &= \pi^{-1}\Psi^2\operatorname{Im}\tilde{\omega}_6^{-1}(E+i0) + O(1),\\
\tilde{\omega}_6(W) &= i\tilde{a}_2^{-1}\left(\mathrm{e}^{2i(\theta-\theta_{-m})}-1\right) - \mathrm{e}^{2i(\theta-\theta_{-m})}\Delta + O\left(\Delta^2\right),\\
\tilde{a}_2 &= \frac{2\sigma}{q^2 m}\left(q_c^2 - \zeta q_c/2 + \sigma^2\right),\\
\Psi &= \sqrt{\frac{q^3 m}{4\sigma^2(q_c^2-\zeta q_c/2+\sigma^2)}},\ \Delta = W+m,\ W \to -m.
\end{aligned}$$

One can see that for $\theta \neq \theta_{-m}$, the function $\sigma'(E)$ is finite for $E = -m$. However, for $\theta = \theta_{-m}$ and for small $E+m$, we have

$$\sigma'(E) = -\pi^{-1}\Psi^2\operatorname{Im}(E+m+i0)^{-1} + O(1) = \Psi^2\delta(E+m) + O(1),$$

that is, there is an eigenvalue $E = -m$ in the spectrum of $\hat{h}_{4,\theta_{-m}}$.

For $-m \leq E < m$ and $K = i\tau = \mathrm{e}^{i\pi/2}\tau$, $\tau = \sqrt{m^2-E^2} > 0$, we have

$$\omega_5(E) = \frac{\Gamma(2i\sigma)\Gamma(-i\sigma-Eq\tau^{-1})\left[\tau(\varkappa+i\sigma)-q(m-E)\right]}{\Gamma(-2i\sigma)\Gamma(i\sigma-Eq\tau^{-1})\left[\tau(\varkappa-i\sigma)-q(m-E)\right]}\left(2\tau m^{-1}\right)^{-2i\sigma}$$

$$\equiv \mathrm{e}^{-2i\Theta(E)},\ \Theta(E) = \sigma\ln\frac{2\tau}{m} + \frac{1}{2i}\{\ln\Gamma(-2i\sigma) - \ln\Gamma(2i\sigma)$$
$$+\ln\Gamma\left(i\sigma - Eq\tau^{-1}\right) - \ln\Gamma\left(-i\sigma - Eq\tau^{-1}\right)$$
$$+\ln\left[\tau(q_{\mathrm{c}} - i\zeta\sigma) - \zeta q(m-E)\right] - \ln\left[\tau(q_{\mathrm{c}} + i\zeta\sigma) - \zeta q(m-E)\right]\},$$

and therefore the function $\omega_6(E) = 4\sigma q^{-1}\tan\left[\Theta(E) - \theta\right]$ is real.

Finally, we obtain

$$\sigma'(E) = \sum_n Q_n^2\delta\left(E - \overset{IV}{E}_n\right),$$
$$Q_n^2 = -\left[\omega_6'\left(\overset{IV}{E}_n\right)\right]^{-1} = -q\left[4\sigma\Theta'\left(\overset{IV}{E}_n\right)\right]^{-1}, \Theta'\left(\overset{IV}{E}_n\right) < 0,$$

so that for $-m \le E < m$, jumps Q_n^2 of the spectral function are located at discrete points $\overset{IV}{E}_n$ defined by the equation

$$\omega_6\left(\overset{IV}{E}_n\right) = 0 \Longrightarrow \sin\left[\Theta\left(\overset{IV}{E}_n\right) - \theta\right] = 0,\ \ \overset{IV}{E}_n = \overset{IV}{E}_n(\theta). \tag{9.51}$$

Thus, the simple spectrum of $\hat{h}_{4,\theta}$ is given by

$$\mathrm{spec}\ \hat{h}_{4,\theta} = \{|E| \ge m\} \cup \left\{\overset{IV}{E}_n\right\}.$$

Some results relating to numerical solution of eq. (9.51) are presented in Figs. 9.2 and 9.3.

The generalized eigenfunctions $U_E(r), |E| \ge m$, and eigenfunctions $U_n(r)$ of $\hat{h}_{4,\theta}$,

$$U_E(r) = \overset{IV}{U}{}_E^{\theta}(r) = \sqrt{\sigma'(E)}U_\theta(r;E),\ |E| \ge m;$$
$$U_n(r) = \overset{IV}{U}{}_n^{\theta}(r) = Q_n U_\theta\left(r;\overset{IV}{E}_n\right), \tag{9.52}$$

form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$.

Let us describe the point spectrum in more detail. To this end, we rewrite (9.51) in the equivalent form

$$\Theta\left(\overset{IV}{E}_n\right) = f(n,\theta) = -\pi l_0 + \pi(-n + \theta/\pi),$$
$$\partial_\theta\overset{IV}{E}_n = \left[\Theta\left(\overset{IV}{E}_n\right)\right]^{-1} < 0, n \in \mathbb{Z}, \tag{9.53}$$

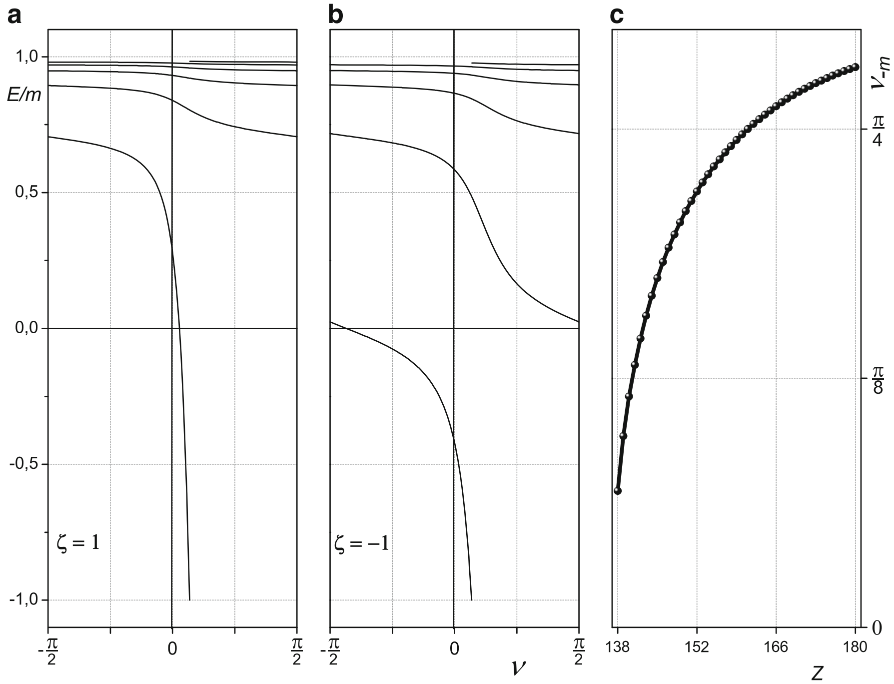

Fig. 9.2 ν-dependence of energy levels $\overset{IV}{E}_n$ for $Z = 138$, $j = 1/2, \zeta = \pm 1$, and Z-dependence of ν_{-m}, $j = 1/2$

where the integer l_0 is defined below. We note that $\Theta(E)$ is a smooth function on the interval $[-m, m)$ and

$$\Theta(E) = -\pi q m^{1/2}[2(m - E)]^{-1/2} + O(1), E \to m - 0.$$

In addition, we have the relation $\Theta(-m) = \theta_{-m} - \pi l_0$, where l_0 is an integer, which follows from the equality

$$\mathrm{e}^{2i\Theta(-m)} = \omega_5^{-1}(-m) = \mathrm{e}^{2i\theta_{-m}}.$$

One can see that the range of the function $f(n, \theta)$, $n \in \mathbb{Z}$, $\theta \in [0, \pi]$, is the whole real axis. This means that for any E, there exist $n \in \mathbb{Z}$, $\theta \in [0, \pi]$ such that $\Theta(E) = f(n, \theta)$. In turn, this means that any $E \in [-m, m)$ is a solution of (9.53) for some n and θ. Therefore, any $E \in [-m, m)$ is the spectrum point for some s.a. Hamiltonian $\hat{h}_{4,\theta}$. As a consequence, we have $\Theta'(E) < 0$, $\forall E \in [-m, m)$. Thus, as E goes from $-m$ to $m - 0$, the function $\Theta(E)$ decreases monotonically from $\theta_{-m} - l_0$ to $-\infty$. One can easily see that in fact, $n \geq 0$ ($n \in \mathbb{Z}_+$). Thus we have the following:

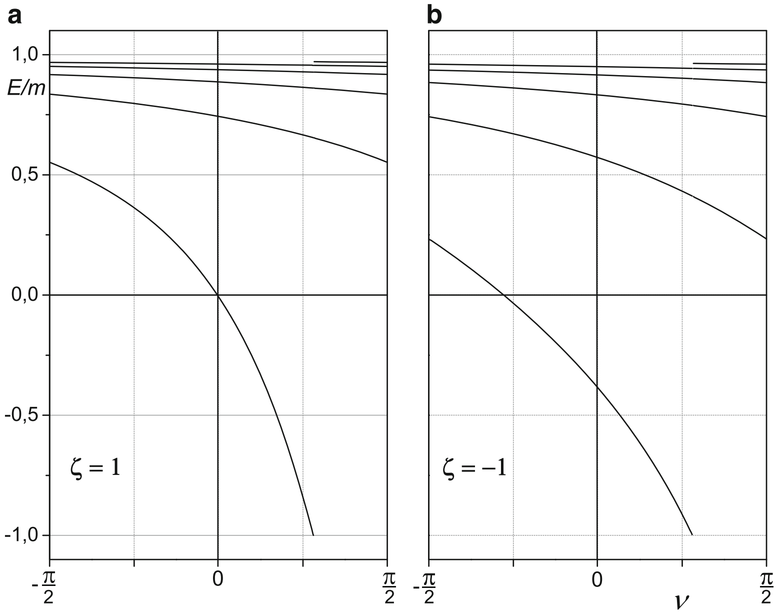

Fig. 9.3 ν-dependence of energy levels $\overset{IV}{E}_n, Z = 180, j = 1/2, \zeta = \pm 1$

(a) in the interval of energies $[-m, \overset{IV}{E}_0(0) = \overset{IV}{E}_1(\pi))$ there are no levels for $\theta \in [\pi/2, \theta_{-m})$, and for any $\theta \in [\theta_{-m}, 0)$, there is one discrete level $\overset{IV}{E}_0(\theta)$, which increases monotonically from $-m$ to $\overset{IV}{E}_0(0) - 0$ as θ goes from θ_{-m} to $+0$;

(b) in each interval of energies $(\overset{IV}{E}_n(\pi), \overset{IV}{E}_n(0) = \overset{IV}{E}_{n+1}(\pi))$, $n \in \mathbb{N}$, there is one discrete level $\overset{IV}{E}_n(\theta)$, which increases monotonically from $\overset{IV}{E}_n(\pi)$ to $\overset{IV}{E}_n(0) - 0$ as θ goes from π to $+0$. In particular, $-m < \overset{IV}{E}_n(0) < \overset{IV}{E}_{n+1}(0) < m$, $\forall n \in \mathbb{Z}_+$.

We note also that there is an infinite number of discrete levels that are accumulated at the point $E = m$. Their asymptotic form as $n \to \infty$ is given by the previous nonrelativistic formula (9.36). The energy of the lower bound state depends essentially on θ, and there exists such an extension parameter θ_{-m} (see (9.50)) for which this energy coincides with the boundary $E = -m$ of the lower continuous spectrum.

9.5 Summary

In Sect. 8.4 we constructed all s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}$ for all values of q (we recall that $q = -q_1 q_2 > 0$, $q_1 = -e$, $q_2 = Ze$, so that $q = Ze^2 = Z\alpha > 0$, and $Z = 137q$ in a hydrogen-like atom) as s.a. extensions of the initial symmetric operators $\hat{h}$ for any j, ζ, and M, and solved spectral problems for all these Hamiltonians. As a result, (10.13) and (9.10) allow one to restore all s.a. Dirac Hamiltonians $\hat{H}_{\mathfrak{e}}$ (all s.a. operators associated with the differential operation (9.1)) for any q and to describe the solution of the corresponding spectral problems for all the Hamiltonians $\hat{H}_{\mathfrak{e}}$.

It is convenient to introduce charge ranges in which the spectral problem has a similar description. These ranges are defined by characteristic points $j_k = k - 1/2$, $k \in \mathbb{Z}_+$, on the axis j of angular momentum eigenvalues. At these points, the functions $q_c(j)$ and $q_s(j)$ are given by

$$q_c(j_k) = k,\ q_c(j_0) = 0,$$
$$q_s(j_{k+1}) = \sqrt{(k+1)^2 - 1/4},\ q_s(j_0) = \sqrt{3}/2,$$

and satisfy the following inequalities:

$$q_c(j_k) < q_s(j_{k+1}) < q_c(j_{k+1}) < q_s(j_{k+2}),\ k \in \mathbb{Z}_+. \tag{9.54}$$

Let us introduce intervals $\Delta(k)$, $k \in \mathbb{Z}_+$, as follows:

$$\Delta(k) = (q_c(j_k), q_c(j_{k+1})] = (k, k+1],\ k \in \mathbb{Z}_+.$$

The semiaxis $(0, \infty)$ can be represented as $(0, \infty) = \cup_{k \in \mathbb{Z}_+} \Delta(k)$. In turn, due to (9.54), each interval $\Delta(k)$ can be represented as $\Delta(k) = \cup_{i=1,2,3} \Delta_i(k)$, where

$$\Delta_1(k) = (q_c(j_k), q_{sc}(j_{k+1})],$$
$$\Delta_2(k) = (q_{sc}(j_{k+1}), q_c(j_{k+1})),$$
$$\Delta_3(k) = \{q_c(j_{k+1})\},\ k \in \mathbb{Z}_+.$$

According to this division, we define three ranges Q_i, $i = 1, 2, 3$, of charges q:

$$Q_i = \cup_{k \in \mathbb{Z}_+} \Delta_i(k),\ i = 1, 2, 3,$$

such that any given $q > 0$ generates a pair of two integers, $k \in \mathbb{Z}_+$ and $i = 1, 2, 3$,

$$q \Longrightarrow (k, i),\ \text{if } q \in Q_i.$$

Then, as follows from the consideration represented in Sects. 9.4.2–9.4.6, we have the following picture.

A. Let $q \Longrightarrow (k, 1)$, that is, $q \in \Delta_1(k)$ for some $k \in \mathbb{Z}_+$, which means that

$$k = q_c(j_k) < q \leq q_{sc}(j_{k+1}) = \sqrt{(k+1)^2 - 1/4}.$$

Consider quantum numbers $j \le j_k$ (such j exist for $k \ge 1$ only). Then $q > q_{\mathrm{c}}(j_k) \ge q_{\mathrm{c}}(j)$, which means that $q > q_{\mathrm{c}}(j)$. Such quantum numbers j are characteristic for the IV range considered in Sect. 9.4.6.

Consider quantum numbers $j \ge j_k + 1$. Then $q \le q_{\mathrm{sc}}(j_k + 1) \le q_{\mathrm{sc}}(j)$. Such quantum numbers j are characteristic for the I range considered in Sect. 9.4.2.

Therefore, for such charges q, we have

$$U_E(r) = \begin{cases} \overset{IV}{U}{}^{\theta}{}_E(r), & j \le j_k, \\ \overset{I}{U}{}_E(r), & j \ge j_k + 1, \end{cases} \qquad |E| \ge m,$$

$$U_n(r) = \begin{cases} \overset{IV}{U}{}^{\theta}{}_n(r), & j \le j_k, \\ \overset{I}{U}{}_n(r), & j \ge j_k + 1, \end{cases} \qquad E_n = \begin{cases} \overset{IV}{E}_n(\theta), & j \le j_k, \\ \overset{I}{E}_n, & j \ge j_k + 1. \end{cases} \tag{9.55}$$

The doublets $\overset{I}{U}_E$ and $\overset{I}{U}_n$ have the form (9.37), and $\overset{IV}{U}{}_E^{\theta}$ and $\overset{IV}{U}{}_n^{\theta}$ have the form (9.52).

The energy spectrum $\overset{I}{E}_n$ is defined by (9.35). The energy spectra $\overset{IV}{E}_n(\theta)$ are defined by (9.51) and (9.53).

B. Let $q \Longrightarrow (k, 2)$, that is, $q \in \Delta_2\,(k)$ for some $k \in \mathbb{Z}_+$, which means that

$$\sqrt{(k+1)^2 - 1/4} = q_{\mathrm{s}}(j_{k+1}) < q < q_{\mathrm{c}}(j_{k+1}) = k + 1.$$

Consider quantum numbers $j \le j_{k+1} - 1 = j_k$ (such j exist for $k \ge 1$ only). Then

$$q > q_{\mathrm{s}}(j_{k+1}) > q_{\mathrm{c}}(j_{k+1} - 1) \ge q_{\mathrm{c}}(j),$$

which means that $q > q_{\mathrm{c}}(j)$. Such quantum numbers j are characteristic for the IV range considered in Sect. 9.4.6.

Consider quantum number $j = j_{k+1}$. In this case $q_{\mathrm{s}}(j) < q < q_{\mathrm{c}}(j)$. Such quantum numbers j are characteristic for the II range considered in Sect. 9.4.4.

Consider quantum numbers $j \ge j_{k+1} + 1 = j_{k+2}$. Then

$$q < q_{\mathrm{c}}(j_{k+1}) < q_{\mathrm{s}}(j_{k+2}) \le q_{\mathrm{sc}}(j),$$

so that $q < q_{\mathrm{s}}(j)$. Such quantum numbers j are characteristic for the I range considered in Sect. 9.4.2.

Therefore, for such charges q, we have

$$U_E(r) = \begin{cases} \overset{IV}{U}{}^{\theta}{}_E(r), & j \le j_k, \\ \overset{II}{U}{}_E^{\nu}(r), & j = j_{k+1}, \\ \overset{I}{U}{}_E(r), & j \ge j_{k+2}, \end{cases} \qquad |E| \ge m,$$

$$U_n(r) = \begin{cases} \overset{IV}{U^{\theta}}_n(r), \ j \le j_k, \\ \overset{II}{U}{}^{\nu}_n(r), \ j = j_{k+1}, \\ \overset{I}{U}_n(r), \ j \ge j_{k+2}, \end{cases} \quad E_n = \begin{cases} \overset{IV}{E}_n(\theta), \ j \le j_k, \\ \overset{II}{E}_n(\nu), \ j = j_{k+1}, \\ \overset{I}{E}_n, \ j \ge j_{k+2}. \end{cases} \tag{9.56}$$

The doublets $\overset{II}{U}{}^{\nu}_E$ and $\overset{II}{U}{}^{\nu}_n$ have the form (9.42), and the energies $\overset{II}{E}_n(\nu)$ are defined by (9.41) and (9.43).

C. Let $q \Longrightarrow (k, 3)$, that is, $q \in \Delta_3(k)$ for some $k \in \mathbb{Z}_+$, which means that

$$q = q_c(j_{k+1}) = k + 1.$$

Consider quantum numbers $j \le j_{k+1} - 1 = j_k$ (such j exist for $k \ge 1$ only). Then

$$q = q_c(j_{k+1}) > q_c(j_{k+1} - 1) \ge q_c(j),$$

so that $q > q_c(j)$. Such quantum numbers j are characteristic for the IV range considered in Sect. 9.4.6.

Consider a quantum number $j = j_{k+1}$. Then $q = q_c(j)$. Such quantum numbers j are characteristic for the III range considered in Sect. 9.4.5.

Consider quantum numbers $j \ge j_{k+1} + 1 = j_{k+2}$. Then

$$q = q_c(j_{k+1}) < q_{sc}(j_{k+1} + 1) \le q_{sc}(j),$$

so that $q < q_{sc}(j)$. Such quantum numbers j are characteristic for the I range considered in Sect. 9.4.2.

Therefore, for such charges, we have

$$U_E(r) = \begin{cases} \overset{IV}{U}{}^{\theta}_E(r), \ j \le j_{k+1} - 1, \\ \overset{III}{U}{}^{\vartheta}_E(r), \ j = j_{k+1}, \\ \overset{I}{U}_E(r), \ j \ge j_{k+1} + 1, \end{cases} \quad |E| \ge m,$$

$$U_n(r) = \begin{cases} \overset{IV}{U}{}^{\theta}_n(r), \ j \le j_{k+1} - 1, \\ \overset{III}{U}{}^{\vartheta}_n(r), \ j = j_{k+1}, \\ \overset{I}{U}_n(r), \ j \ge j_{k+1} + 1, \end{cases} \quad E_n = \begin{cases} \overset{IV}{E}_n(\theta), \ j \le j_{k+1} - 1, \\ \overset{III}{E}_n(\vartheta), \ j = j_{k+1} \ \overset{I}{E}_n, \ j \ge j_{k+1} + 1. \end{cases} \tag{9.57}$$

The doublets $\overset{III}{U}{}^{\vartheta}_E$ and $\overset{III}{U}{}^{\vartheta}_n$ have the form (9.47), and the energies $\overset{III}{E}_n(\vartheta)$ are defined by (9.46) and (9.48).

We are now in a position to describe the spectral problem for all the s.a. Dirac Hamiltonians with any charge q. Consider eigenvectors $\Psi_{j,M,\zeta,E}(\mathbf{r})$ of any s.a. Dirac Hamiltonian $\hat{H}_{\mathfrak{e}}$. They satisfy the following set of equations (see Sect. 9.2):

$$\begin{aligned}
\check{H}\Psi_{j,M,\zeta,E}(\mathbf{r}) &= E\Psi_{j,M,\zeta,E}(\mathbf{r}),\\
\hat{\mathbf{J}}^2\Psi_{j,M,\zeta}(\mathbf{r}) &= j(j+1)\Psi_{j,M,\zeta}(\mathbf{r}),\ j = k + 1/2,\ k \in \mathbb{Z}_+,\\
\hat{J}_z\Psi_{j,M,\zeta}(\mathbf{r}) &= M\Psi_{j,M,\zeta},\ M = -j, -j+1, \dots, j-1, j,\\
\hat{K}\Psi_{j,M,\zeta}(\mathbf{r}) &= -\zeta(j+1/2)\Psi_{j,M,\zeta}(\mathbf{r}),\ \zeta = \pm 1,
\end{aligned}$$

where the Dirac differential operation is $\check{H}$, and operators $\hat{\mathbf{J}}^2$, $\hat{J}_z$, and $\hat{K}$, are given by (9.1) and (9.2), whereas the eigenvectors have the form $\Psi_{j,M,\zeta,E}(\mathbf{r}) = \mathbf{\Pi}_{j,M,\zeta}U_E(r)$, see (9.7).

For any charge q, the energy spectrum of any s.a. Dirac Hamiltonian $\hat{H}_{\mathfrak{e}}$ consists of the continuous part $|E| \geq m$ and a discrete part E_n, which is placed in the interval $[-m, m)$.

The eigenvectors $\Psi_{j,M,\zeta,E}(\mathbf{r})$, $|E| \geq m$, which correspond to the continuous part of the spectrum, are generalized eigenvectors of $\hat{H}_{\mathfrak{e}}$, whereas the eigenvectors $\Psi_{j,M,\zeta,E_n}(\mathbf{r})$ of $\hat{H}_{\mathfrak{e}}$, which correspond to the discrete part of the spectrum, belong to the Hilbert space $\boldsymbol{L}^2(\mathbb{R}^3)$. Doublets $U_E(r)$, which belong to the discrete energies E_n, are denoted by $U_{E_n}(r) = U_n(r)$. All the doublets $U_E(r)$ and $U_n(r)$ and the spectra E_n depend on the extension parameters, on the quantum numbers j, M, and ζ, and on the charge q according to (9.55), (9.56), and (9.57). It should be remembered that the extension parameters depend on both j and ζ.

Finally, the total s.a. Dirac Hamiltonian $\hat{H}(Z)$ with $Z \leq 118$ is defined uniquely. For $Z \geq 119$, there is a family of possible total s.a. Dirac Hamiltonians. The family is parameterized by the extension parameters. The number of the extension parameters is equal to $2k(Z)$, where $k(Z) = (1/4 + Z^2\alpha^2)^{1/2} - \delta$ is an integer and $0 < \delta \leq 1$. For $Z \geq 119$, any specific s.a. Dirac Hamiltonian $\hat{H}(Z)$ corresponds to a certain prescription for the behavior of an electron at the origin. The general theory thus describes all the possibilities that can be offered to a physicist. Which to choose is a completely physical problem.

We believe that each s.a. Dirac Hamiltonian with superstrong Coulomb field can be understood through an appropriate regularization of the potential and a subsequent limit process of removing the regularization. We recall that a physical interest in the electronic structure of superheavy atoms was mainly motivated by a possible pair creation in the superstrong Coulomb field. Consideration of this effect in the framework of the simplest model of a pointlike nucleus was considered impossible due to the conclusion (which is wrong, as is now clear) that this model is mathematically inconsistent [166]. We believe that the described rehabilitation of the model allows a return to a consideration of particle creation in this model, which provides great scope for analytical studies.

Chapter 10
Schrödinger and Dirac Operators with Aharonov–Bohm and Magnetic-Solenoid Fields

10.1 Introduction

10.1.1 General Remarks

The *Aharonov–Bohm (AB) effect* plays an important role in QT, revealing a peculiar status of electromagnetic potentials in the theory [89, 120, 124]. This effect was discussed in [6] in relation to the scattering of a nonrelativistic charged spinless particle by an infinitely long and infinitely thin magnetic field of a solenoid (the *AB field* in what follows) of finite magnetic flux (a similar effect was discussed earlier by Ehrenberg and Siday [53]). It was found that a particle wave function vanishes at the solenoid line. Although the particle does not penetrate the solenoid, while the magnetic field vanishes outside of it, the partial scattering phases are proportional to the magnetic flux (modulo a flux quantum) [165].

A nontrivial particle scattering by such a field was interpreted as a capability of a quantum particle to "feel" an electromagnetic field vector potential because the AB field vector potential does not vanish outside of the solenoid.[1] An s.a. nonrelativistic Hamiltonian with the AB field was first constructed in [150]; see also [33, 135]. The problem of s.a. extensions of Dirac operators with the AB field in $2+1$ dimensions was first recognized in [72, 73, 85]. Self-adjoint Dirac Hamiltonians with the AB field in $3+1$ dimensions were constructed in [10, 40, 42, 159]. In all these cases, s.a. Hamiltonians are specified by s.a. boundary conditions on the solenoid line. One possible boundary condition was obtained in [4, 58, 85] by a specific regularization of the Dirac delta function, starting from a model in which the continuity of both components of the Dirac spinor is imposed at a finite radius, and then this radius is shrunk to zero; see also [2, 121]. Physically

[1] It should be mentioned that in the relativistic case (Dirac equation with AB field) some of the wave functions from a complete set of solutions do not vanish on the solenoid line.

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motivated boundary conditions for particle scattering by a superposition of the AB field and a Coulomb field were studied in [41, 86, 152]. A splitting of Landau levels in a superposition of the AB field and a parallel uniform magnetic field gives an example of the AB effect for bound states. In what follows, we call such a superposition the *magnetic-solenoid field* (*MSF*). Solutions of the nonrelativistic stationary Schrödinger equation with MSF were first studied in [107]. Solutions of the relativistic wave equations (Klein–Gordon and Dirac) with MSF were first obtained in [15] and then used to study the AB effect in cyclotron and synchrotron radiations in [16–18]. On the basis of these solutions, the problem of the self-adjointness of Dirac Hamiltonians with MSF was studied in [66–69]. Coherent states in MSF were constructed in [14]. A complete spectral analysis for all the s.a. nonrelativistic and relativistic Hamiltonians with MSF was performed in [78]. Recently, interest in such a superposition has been renewed in connection with planar physics problems and the quantum Hall effect [55, 110, 117].

In this chapter, we construct all the s.a. relativistic and nonrelativistic Hamiltonians with MSF and solve the corresponding spectral problems.

10.1.2 AB and Magnetic-Solenoid Fields

The AB field of an infinitely thin solenoid (with constant flux $\varPhi$) along the axis $z = x^3$ can be described by the electromagnetic potentials $A^{\mu}_{\mathrm{AB}}, \mu = 0, 1, 2, 3,$

$$A^{\mu}_{\mathrm{AB}} = (0, \mathbf{A}_{\mathrm{AB}}), \mathbf{A}_{\mathrm{AB}} = \left(A^{k}_{\mathrm{AB}},\ k = 1, 2, 3\right), A^{3}_{\mathrm{AB}} = 0,$$
$$A^{1}_{\mathrm{AB}} = -\frac{\varPhi \sin\varphi}{2\pi\rho}, A^{2}_{\mathrm{AB}} = \frac{\varPhi \cos\varphi}{2\pi\rho},$$

where ρ, φ are cylindrical coordinates, $x^1 = x = \rho\cos\varphi, x^2 = y = \rho\sin\varphi$, and $\rho = \sqrt{x^2 + y^2}$.

The magnetic field of an AB solenoid has the form $\mathbf{B}_{\mathrm{AB}} = (0, 0, B_{\mathrm{AB}})$. It is easy to see that outside the z-axis, the magnetic field $\mathbf{B}_{\mathrm{AB}} = \mathrm{rot}\mathbf{A}_{\mathrm{AB}}$ is equal to zero. Nevertheless, for any surface $\varSigma$ with boundary L that is any contour (even an infinitely small one) around the z-axis, the circulation of the vector potential along L does not vanish and reads $\oint_L \mathbf{A}_{\mathrm{AB}} d\mathbf{l} = \varPhi$. If one interprets this circulation as the flux of the magnetic field $\mathbf{B}_{\mathrm{AB}}$ through the surface $\varSigma$,

$$\int_{\varSigma} \mathbf{B}_{\mathrm{AB}} d\sigma = \oint_L \mathbf{A}_{\mathrm{AB}} d\mathbf{l} = \varPhi,$$

then we obtain an expression for the magnetic field,

$$B_{\mathrm{AB}} = \varPhi\delta\left(x^1\right)\delta\left(x^2\right),$$

which is the origin of the term “infinitely thin solenoid”.

One can see that $\mathbf{A}_{\mathrm{AB}} = -\mathrm{rot}\Psi,\ \Psi = (0, 0, \frac{\Phi}{2\pi} \ln \rho)$, so that $\mathrm{div}\mathbf{A}_{\mathrm{AB}} = 0$, and again

$$\mathbf{B}_{\mathrm{AB}} = \mathrm{rot}\mathbf{A}_{\mathrm{AB}} = (0, 0, B_{\mathrm{AB}}),\ B_{\mathrm{AB}} = \frac{\Phi}{2\pi} \Delta \ln \rho = \Phi \delta\left(x^1\right) \delta\left(x^2\right).$$

We have

$$\frac{e}{c\hbar} A^1_{\mathrm{AB}} = -\phi\rho^{-1} \sin\varphi\,,\ \frac{e}{c\hbar} A^2_{\mathrm{AB}} = \phi\rho^{-1} \cos\varphi,$$

where $\phi = \Phi/\Phi_0$, and Φ_0 is *a fundamental unit of magnetic flux*, [46, 47],

$$\Phi_0 = 2\pi c\hbar/e = 4.135 \times 10^{-7}\,\mathrm{G} \cdot \mathrm{cm}^2$$

(we recall that $e > 0$ is the absolute value of the electron charge).

As already mentioned, the MSF is defined as a superposition of a constant uniform magnetic field of strength B directed along the z-axis and the AB field with the flux Φ in the same direction. The MSF can be described by electromagnetic potentials of the form $A^\mu = (0, \mathbf{A})$, $\mathbf{A} = \left(A^k,\ k = 1, 2, 3\right)$,

$$A^1 = A^1_{\mathrm{AB}} - \frac{Bx^2}{2},\ A^2 = A^2_{\mathrm{AB}} + \frac{Bx^1}{2},\ A^3 = 0. \tag{10.1}$$

The potentials (10.1) define the magnetic field $\mathbf{B} = (0, 0, B + B_{\mathrm{AB}})$. Such a magnetic field is called MSF. In cylindrical coordinates, the potentials of the MSF have the form

$$\frac{e}{c\hbar} A^1 = -\tilde{\phi}\rho^{-1} \sin\varphi, \frac{e}{c\hbar} A^2 = \tilde{\phi}\rho^{-1} \cos\varphi, A^3 = 0,$$
$$\tilde{\phi} = \phi + \frac{\epsilon_B \gamma \rho^2}{2}, \gamma = \frac{e|B|}{c\hbar} > 0, \epsilon_B = \mathrm{sgn}\ B. \tag{10.2}$$

Below, we consider nonrelativistic and relativistic quantum Hamiltonians of a charged particle of mass m_e and charge $q = \epsilon_q e, \epsilon_q = \mathrm{sgn}\, q = \pm 1$ (positron or electron) in the AB field and the MSF.

For further consideration, it is convenient to represent the dimensionless quantity $q\Phi(2\pi c\hbar)^{-1}$ as follows:

$$\frac{q\Phi}{2\pi c\hbar} = \epsilon_q \frac{\Phi}{\Phi_0} = \epsilon_q \phi = \epsilon(\phi_0 + \mu) \Longleftrightarrow \phi = \epsilon_B\left(\phi_0 + \mu\right),$$

$$\epsilon = \epsilon_q \epsilon_B = \mathrm{sgn}\ (qB)\,,\ \phi_0 = [\epsilon_B \phi] \in \mathbb{Z},\ \mu = \epsilon_B \phi - \phi_0,\ 0 \le \mu < 1.$$

The quantity μ is called the mantissa of the magnetic flux, and in fact, it determines all the quantum effects in the AB field; see, for example [17].

10.2 Self-adjoint Schrödinger Operators

In this section, we consider two-dimensional and three-dimensional Schrödinger operators with AB and MSF. The starting point is the s.a. differential Schrödinger operation $\check{H}$ with MSF. In three dimensions, it is given by the expression

$$\check{H} = \frac{1}{2m_e}\left(\check{\mathbf{p}} - \frac{q}{c}\mathbf{A}\right)^2, \check{\mathbf{p}} = -i\hbar\nabla, \nabla = \left(\partial_x, \partial_y, \partial_z\right). \tag{10.3}$$

It is convenient to represent $\check{H}$ as a sum of two terms, $\check{H}^{\perp}$ and $\check{H}^{\parallel}$,

$$\check{H} = \check{H}^{\perp} + \check{H}^{\parallel},$$

where the two-dimensional s.a. differential Schrödinger operation $\check{H}^{\perp}$ with the MSF,

$$\begin{aligned} &\check{H}^{\perp} = M^{-1}\check{\mathcal{H}}^{\perp},\ \check{\mathcal{H}}^{\perp} = \left(-i\nabla^{\perp} - \frac{q}{c\hbar}\mathbf{A}^{\perp}\right)^2, \\ &M = 2m_e\hbar^{-2}, \nabla^{\perp} = \left(\partial_x, \partial_y\right), \mathbf{A}^{\perp} = \left(A^1, A^2\right), \end{aligned} \tag{10.4}$$

A^1 and A^2 are given by (10.2), corresponds to a two-dimensional motion in the xy-plane, while the one-dimensional differential operation $\check{H}^{\parallel}$,

$$\check{H}^{\parallel} = \check{\mathcal{H}} = \frac{\check{p}_z^2}{2m_e}, \check{p}_z = -i\hbar\partial_z,$$

corresponds to a one-dimensional free motion along the z-axis.

The problem to be solved is to construct two- and three-dimensional s.a. Hamiltonians $\hat{H}^{\perp}$ and $\hat{H}$ associated with the respective s.a. differential operations $\check{H}^{\perp}$ and $\check{H}$ and to perform a complete spectral analysis for these operators.

We begin with the two-dimensional problem. We successively consider the case of a pure AB field, with $B = 0$, and then the case of the MSF. Then, we generalize and obtain results in three dimensions.

10.2.1 Two-Dimensional Case

10.2.1.1 Reduction to Radial Problem

In the case of two dimensions, the space of the particle quantum states is the Hilbert space $\mathfrak{H} = L^2\left(\mathbb{R}^2\right)$ of square-integrable functions $\psi(\rho)$, $\rho = (x, y)$, with the scalar product

$$(\psi_1, \psi_2) = \int \overline{\psi_1(\rho)}\psi_2(\rho)\mathrm{d}\rho,\ \mathrm{d}\rho = \mathrm{d}x\,\mathrm{d}y = \rho\,\mathrm{d}\rho\,\mathrm{d}\varphi.$$

A quantum Hamiltonian should be defined as an s.a. operator in this Hilbert space. It is more convenient to deal with s.a. operators associated with the s.a. differential operation $\check{\mathcal{H}}^{\perp} = M\check{H}^{\perp}$ defined in (10.4).

The construction is essentially based on the requirement of rotational symmetry, which certainly holds in a classical description of the system. This requirement is formulated as the requirement of the invariance of an s.a. Hamiltonian under rotations around the solenoid line, the z-axis. As in classical mechanics, the rotational symmetry makes it possible to separate the polar coordinates ρ and φ and reduce the two-dimensional problem to a one-dimensional radial problem.

The group of rotations $SO(2)$ in $\mathbb{R}^2$ naturally acts in the Hilbert space $\mathfrak{H}$ by unitary operators: if $S \in SO(2)$, then the corresponding operator $\hat{U}_S$ is defined by the relation $\left(\hat{U}_S\psi\right)(\rho) = \psi\left(S^{-1}\rho\right), \psi \in \mathfrak{H}$.

The Hilbert space $\mathfrak{H}$ is a direct orthogonal sum of subspaces $\mathfrak{H}_m$ that are the eigenspaces of the representation $\hat{U}_S$,

$$\mathfrak{H} = \sum_{m\in\mathbb{Z}}^{\oplus} \mathfrak{H}_m,\ \hat{U}_S\mathfrak{H}_m = \mathrm{e}^{-im\theta}\mathfrak{H}_m,$$

where θ is the rotation angle corresponding to S.

It should be noted that $\mathfrak{H}_m$ consists of eigenfunctions $\psi_m(\rho)$ for the angular momentum operator $\hat{L}_z = -i\hbar\partial/\partial\varphi$,

$$\hat{L}_z\psi_m(\rho) = \hbar m\psi_m(\rho),\ \psi_m(\rho) = \frac{1}{\sqrt{2\pi\rho}}\mathrm{e}^{im\varphi} f_m(\rho),\ \forall\psi_m \in \mathfrak{H}_m.$$

It is convenient to change the indexing, $m \to l$, $\mathfrak{H}_m \to \mathfrak{H}_l$, $\psi_m(\rho) \to \psi_l(\rho)$, as follows $m = \epsilon(\phi_0 - l)$, so that

$$\hat{L}_z\psi_l(\rho) = \hbar\epsilon(\phi_0 - l)\psi_l(\rho),\ \forall\psi_l \in \mathfrak{H}_l.$$

We define a rotationally invariant initial symmetric operator $\widehat{\mathcal{H}}^{\perp}$ associated with $\check{\mathcal{H}}^{\perp}$ as follows:

$$\widehat{\mathcal{H}}^{\perp} : \begin{cases} D_{\mathcal{H}^{\perp}} = \left\{\psi(\rho) : \psi \in \mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right)\right\}, \\ \widehat{\mathcal{H}}^{\perp}\psi = \check{\mathcal{H}}^{\perp}\psi,\ \forall\psi \in D_{\mathcal{H}^{\perp}}, \end{cases}$$

where $\mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right)$ is the space of smooth and compactly supported functions vanishing in a neighborhood of the point $\boldsymbol{æ} = 0$. The domain $D_{\mathcal{H}^{\perp}}$ is dense in $\mathfrak{H}$, and the symmetry of $\widehat{\mathcal{H}}^{\perp}$ is obvious.

In polar coordinates ρ and φ, the operation $\check{\mathcal{H}}^{\perp}$ becomes

$$\check{\mathcal{H}}^{\perp} = -\partial_\rho^2 - \rho^{-1}\partial_\rho + \rho^{-2}\left(i\partial_\varphi + \epsilon_q\tilde{\phi}\right)^2, \tag{10.5}$$

where $\tilde{\phi}$ is given by (10.2).

For every l, the relation

$$(S_l f)(\rho) = \psi_l(\rho) = \frac{1}{\sqrt{2\pi\rho}} e^{i\epsilon(\phi_0 - l)\varphi} f_l(\rho), \tag{10.6}$$

where $f = f(\rho) \in L^2(\mathbb{R}_+)$ and $f_l(\rho) = f(\rho)$, determines a unitary operator $S_l \colon L^2(\mathbb{R}_+) \longmapsto \mathfrak{H}_l$, where $L^2(\mathbb{R}_+)$ is the Hilbert space of square-integrable functions on the semiaxis $\mathbb{R}_+$ with scalar product

$$(f, g) = \int_{\mathbb{R}_+} \overline{f(\rho)} g(\rho) \, d\rho.$$

For every l, we define a linear operator V_l from $\mathfrak{H}$ to $L^2(\mathbb{R}_+)$ by setting

$$(V_l \psi)(\rho) = \sqrt{\frac{\rho}{2\pi}} \int_0^{2\pi} \psi(\rho, \varphi) e^{-i\epsilon(\phi_0 - l)\varphi} d\varphi. \tag{10.7}$$

If $\psi \in \mathfrak{H} = \sum_{l \in \mathbb{Z}} \psi_l$, $\psi_l \in \mathfrak{H}_l$, then we have $\psi_l = S_l V_l \psi$ for all l. In other words, $V_l = S_l^{-1} P_l$, where P_l is the orthogonal projector onto the subspace $\mathfrak{H}_l$. However, we prefer to work with V_l rather than P_l because the latter cannot be reasonably defined in the three-dimensional case, where the Hilbert state space should be decomposed into a direct integral instead of a direct sum (see Sects. 10.2.2 and 10.4).

Clearly, $V_l \psi \in \mathcal{D}(\mathbb{R}_+)$ for any $\psi \in \mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right)$, and it follows from (10.5) and (10.7) that

$$V_l \widehat{\mathcal{H}}^{\perp} \psi = \hat{h}(l) V_l \psi, \;\; \psi \in \mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right), \tag{10.8}$$

where the initial symmetric operator $\hat{h}(l)$ is defined on $D_{h(l)} = \mathcal{D}(\mathbb{R}_+) \subset L^2(\mathbb{R}_+)$, where it acts as

$$\check{h}(l) = -\partial_\rho^2 + \rho^{-2}\left[\left(l + \mu + \gamma\rho^2/2\right)^2 - 1/4\right]. \tag{10.9}$$

In view of (10.8), for any $\psi \in \mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right)$, the $\mathfrak{H}_l$-component $\left(\widehat{\mathcal{H}}^{\perp}\psi\right)_l$ of $\widehat{\mathcal{H}}^{\perp}\psi$ can be written as

$$\left(\widehat{\mathcal{H}}^{\perp}\psi\right)_l = S_l V_l \widehat{\mathcal{H}}^{\perp}\psi = S_l \hat{h}(l) S_l^{-1} S_l V_l \psi = S_l \hat{h}(l) S_l^{-1} \psi_l. \tag{10.10}$$

Suppose we have a (not necessarily closed) operator $\hat{f}_l$ in $\mathfrak{H}_l$ for each l. We define the operator

$$\hat{f} = \sum_{l \in \mathbb{Z}}^{\oplus} \hat{f}_l \tag{10.11}$$

in $\mathfrak{H}$ by setting

$$\hat{f}\psi = \sum_{l\in\mathbb{Z}} \hat{f}_l \psi_l, \ \psi = \sum_{l\in\mathbb{Z}} \psi_l.$$

The domain D_f of $\hat{f}$ consists of all $\psi = \sum_{l\in\mathbb{Z}} \psi_l \in \mathfrak{H}$ such that $\psi_l \in D_{f_l}$ for all l and the series $\sum_{l\in\mathbb{Z}} \hat{f}_l \psi_l$ converges in $\mathfrak{H}$. The operator $\hat{f}$ is closed (s.a.) iff all $\hat{f}_l$ are closed (respectively, s.a.). For every l, we have $D_{f_l} = D_f \cap \mathfrak{H}_l$.

We say that a closed operator $\hat{f}$ in $\mathfrak{H}$ is *rotationally invariant* if it can be represented in the form (10.11) for some family of operators $\hat{f}_l$ in $\mathfrak{H}_l$.

By (10.10), the direct sum of the operators $S_l \hat{h}(l) S_l^{-1}$ is an extension of $\widehat{\mathcal{H}}^{\perp}$:

$$\widehat{\mathcal{H}}^{\perp} \subseteq \sum_{l\in\mathbb{Z}}^{\oplus} S_l \hat{h}(l) S_l^{-1}. \tag{10.12}$$

Let $\hat{h}_{\mathfrak{e}}(l)$ be s.a. extensions of the symmetric operators $\hat{h}(l)$. Then the operators

$$\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l) = S_l \hat{h}_{\mathfrak{e}}(l) S_l^{-1} \tag{10.13}$$

are s.a. extensions of $S_l \hat{h}(l) S_l^{-1}$, and it follows from (10.12) that the orthogonal direct sum

$$\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp} = \sum_{l\in\mathbb{Z}}^{\oplus} \widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l) \tag{10.14}$$

represents rotationally invariant s.a. extensions of the initial operator $\widehat{\mathcal{H}}^{\perp}$.

Conversely, let $\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}$ be a rotationally invariant s.a. extension of $\widehat{\mathcal{H}}^{\perp}$. Then it has the form (10.14), where $\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l)$ are s.a. operators in $\mathfrak{H}_l$. Let us set $\hat{h}_{\mathfrak{e}}(l) = S_l^{-1} \widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l) S_l$. For all l, $\hat{h}_{\mathfrak{e}}(l)$ are s.a. operators in $L^2(\mathbb{R}_+)$. If $f \in \mathcal{D}(\mathbb{R}_+)$, then $S_l f \in \mathcal{D}\left(\mathbb{R}^2 \setminus \{0\}\right) \cap \mathfrak{H}_l$ and (10.12) and (10.14) imply that

$$S_l \hat{h}(l) f = S_l \hat{h}(l) S_l^{-1} S_l f = \widehat{\mathcal{H}}^{\perp} S_l f = \widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp} S_l f = \widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l) S_l f = S_l \hat{h}_{\mathfrak{e}}(l) f.$$

Hence, $\hat{h}(l) f = \hat{h}_{\mathfrak{e}}(l) f$, that is, $\hat{h}_{\mathfrak{e}}(l)$ is an s.a. extension of $\hat{h}(l)$. We thus conclude that $\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}$ can be represented in the form (10.14), where $\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}(l)$ are given by (10.13) and $\hat{h}_{\mathfrak{e}}(l)$ are s.a. extensions of $\hat{h}(l)$.

The problem of constructing a rotationally invariant s.a. Hamiltonian $\widehat{\mathcal{H}}_{\mathfrak{e}}^{\perp}$ is thus reduced to constructing s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(l)$. We first consider the case of a pure AB field where $B = 0$. In such a case, we set $\epsilon_B = 1$ and $\epsilon = \epsilon_q$.

10.2.1.2 Self-adjoint Radial Hamiltonians with Pure AB Field

In this case, we have $\gamma = 0$, and s.a. radial differential operations $\check{h}(l)$ (10.9) become

$$\check{h}\,(l) = -\partial_\rho^2 + \alpha\rho^{-2},\;\; \alpha = \varkappa_l^2 - 1/4,\;\; \varkappa_l = |l+\mu|,\; l \in \mathbb{Z}.$$

It is easy to see that these differential operations and the corresponding initial symmetric operators $\hat{h}\,(l)$ are actually identical to the respective operations and operators encountered in studying the Calogero problem in Sect. 7.2. We can therefore directly carry over the previously obtained results to s.a. extensions of $\hat{h}\,(l)$.

First Region: $\alpha \geq 3/4$

In this region, we have $(l+\mu)^2 \geq 1$, which is equivalent to $l \geq 1-\mu$ or $l \leq -1-\mu$. Because $l \in \mathbb{Z}$ and $0 \leq \mu < 1$, we have to distinguish the cases of $\mu = 0$ and $\mu > 0$:

$$\mu = 0 : l \leq -1 \text{ or } l \geq 1,\; \text{i.e.,}\;\; l \neq 0,$$
$$\mu > 0 : l \leq -2 \text{ or } l \geq 1,\; \text{i.e.,}\;\; l \neq 0, -1.$$

For such l, the initial symmetric operator $\hat{h}\,(l)$ has zero deficiency indices, is essentially s.a., and its unique s.a. extension is $\hat{h}_1\,(l) = \hat{h}^+\,(l)$ with domain $D^*_{\check{h}(l)}\,(\mathbb{R}_+)$. The spectrum of $\hat{h}_{(1)}\,(l)$ is simple and continuous and coincides with the positive semiaxis, spec $\hat{h}_1\,(l) = \mathbb{R}_+$.

The generalized eigenfunctions $U_{\mathcal{E}}$,

$$U_{\mathcal{E}}(\rho) = (\rho/2)^{1/2}\, J_{\varkappa_l}\left(\sqrt{\mathcal{E}}\rho\right),$$

of $\hat{h}_1\,(l)$ form a complete orthonormalized system in $L^2(\mathbb{R}_+)$.

Second Region: $-1/4 < \alpha < 3/4$

In this region, we have $0 < (l+\mu)^2 < 1$, which is equivalent to

$$-\mu < l < 1-\mu \text{ or } -1-\mu < l < -\mu. \tag{10.15}$$

If $\mu = 0$, inequalities (10.15) have no solutions for $l \in \mathbb{Z}$. If $\mu > 0$, these inequalities have two solutions $l = l_a$, $a = 0, -1$, where for brevity, we introduce the notation $l_a = a$, $a = 0, -1$. So in the second region, we remain with the case $\mu > 0$.

For each $l = l_a$, there exists a one-parameter $U(1)$ family of s.a. radial Hamiltonians $\hat{h}_{\lambda_a}(l_a)$ parameterized by the real parameter $\lambda_a \in \mathbb{S}(-\pi/2, \pi/2)$. These Hamiltonians are specified by the asymptotic s.a. boundary conditions at $\rho \to 0$,

$$\psi_{\lambda_a}(\rho) = C\left[(\kappa_0\rho)^{1/2+\varkappa_a}\cos\lambda_a + (\kappa_0\rho)^{1/2-\varkappa_a}\sin\lambda_a\right] + O\left(\rho^{3/2}\right), \qquad (10.16)$$

such that

$$D_{h_{\lambda_a}(l_a)} = \left\{\psi : \psi \in D^*_{\check{h}(l_a)}(\mathbb{R}_+),\ \psi \text{ satisfy } (10.16)\right\},$$

where $\varkappa_a \equiv \varkappa_{l_a} = |\mu + a|, 0 < \varkappa_a < 1$, and C is an arbitrary constant, whereas k_0 is a constant of dimension of inverse length.

For $\lambda_a \notin (-\pi/2, 0)$, the spectrum of each $\hat{h}_{\lambda_a}(l_a)$ is simple and continuous, and spec $\hat{h}_{\lambda_a}(l_a) = \mathbb{R}_+$.

The generalized eigenfunctions $U_{\mathcal{E}}$,

$$\begin{aligned}
U_{\mathcal{E}}(\rho) &= \sqrt{\frac{\rho}{2Q_a}}\left[J_{\varkappa_a}\left(\sqrt{\mathcal{E}}\rho\right) + \tilde{\lambda}_a\left(\sqrt{\mathcal{E}}/2\kappa_0\right)^{2\varkappa_a} J_{-\varkappa_a}\left(\sqrt{\mathcal{E}}\rho\right)\right],\\
Q_a &= 1 + 2\tilde{\lambda}_a(\mathcal{E}/4)^{\varkappa_a}\cos(\pi\varkappa_a) + \left(\tilde{\lambda}_a\right)^2(\mathcal{E}/4)^{2\varkappa_a} > 0,\\
\tilde{\lambda}_a &= \Gamma(1-\varkappa_a)\Gamma^{-1}(1+\varkappa_a)\tan\lambda_a\,,
\end{aligned} \qquad (10.17)$$

of the Hamiltonian $\hat{h}_{\lambda_a}(l_a)$ form a complete orthonormalized system in the Hilbert space $L^2(\mathbb{R}_+)$.

For $\lambda_a \in (-\pi/2, 0)$, the spectrum of each of $\hat{h}_{\lambda_a}(l_a)$ is simple, but in addition to the continuous part of the spectrum, there exists one negative level $\mathcal{E}^{(-)}_{\lambda_a} = -4k_0^2\left|\tilde{\lambda}_a\right|^{-\varkappa_a^{-1}}$, so that the simple spectrum of $\hat{h}_{\lambda_a}(l_a)$ is given by spec $\hat{h}_{\lambda_a}(l_a) = \mathbb{R}_+ \cup \left\{\mathcal{E}^{(-)}_{\lambda_a}\right\}$.

In this case, the generalized eigenfunctions $U_{\mathcal{E}}$ of the continuous spectrum, $\mathcal{E} \geq 0$, are given by the same (10.17), while the eigenfunction $U^{(-)}$ corresponding to the discrete level $\mathcal{E}^{(-)}_{\lambda_a}$ is

$$U^{(-)}(\rho) = \sqrt{\frac{2\rho\left|\mathcal{E}^{(-)}_{\lambda_a}\right|\sin(\pi\varkappa_a)}{\pi\varkappa_a}}K_{\varkappa_a}\left(\sqrt{\left|\mathcal{E}^{(-)}_{\lambda_a}\right|}\rho\right).$$

They together form a complete orthonormalized system in each Hilbert space $L^2(\mathbb{R}_+)$.

Third Region: $\alpha = -1/4$

In this region, we have $l + \mu = 0$. If $\mu = 0$, this equation has a unique solution $l = l_0 = 0$, while if $\mu > 0$, there are no solutions, and we remain with the only case, $\mu = 0$.

For $l = l_0$, there exists a one-parameter $U(1)$ family of s.a. radial Hamiltonians $\hat{h}_\lambda(l_0)$, parameterized by the real parameter $\lambda \in \mathbb{S}(-\pi/2, \pi/2)$. These Hamiltonians are specified by the asymptotic s.a. boundary conditions at $\rho \to 0$,

$$\psi_\lambda(\rho) = C\left[\rho^{1/2}\ln(\kappa_0\rho)\cos\lambda + \rho^{1/2}\sin\lambda\right] + O\left(\rho^{3/2}\ln\rho\right), \tag{10.18}$$

such that

$$D_{h_\lambda(l_0)} = \left\{\psi : \ \psi \in D^*_{\check{h}(l_0)}(\mathbb{R}_+), \ \psi \text{ satisfy } (10.18)\right\},$$

where the constants C and k_0 are of the same meaning as in (10.16).

The spectrum of $\hat{h}_\lambda(l_0)$ is simple. For $|\lambda| = \pi/2$, the simple spectrum is given by spec $\hat{h}_{\pm\pi/2}(l_0) = \mathbb{R}_+$. For $|\lambda| < \pi/2$, in addition to the continuous part of the spectrum, there exists one negative level $\mathcal{E}_\lambda^{(-)} = -4\kappa_0^2\exp\left[2(\tan\lambda - \mathbf{C})\right]$, where $\mathbf{C}$ is Euler's constant, such that

$$\operatorname{spec}\hat{h}_\lambda(l_0) = \mathbb{R}_+ \cup \left\{\mathcal{E}_\lambda^{(-)}\right\}, \ |\lambda| < \pi/2.$$

The generalized eigenfunctions $U_\mathcal{E}$ of the continuous spectrum,

$$U_\mathcal{E}(\rho) = \sqrt{\frac{\rho}{2\left(\tilde{\lambda}^2 + \pi^2/4\right)}}\left[\tilde{\lambda}J_0\left(\sqrt{\mathcal{E}}\rho\right) + \frac{\pi}{2}N_0\left(\sqrt{\mathcal{E}}\rho\right)\right],$$

$$\tilde{\lambda} = \tan\lambda - \mathbf{C} - \ln\left(\sqrt{\mathcal{E}}/2\kappa_0\right), \ |\lambda| \leq \pi/2,$$

and the eigenfunction $U^{(-)}$ corresponding to the discrete level,

$$U^{(-)}(\rho) = \sqrt{2\rho\left|\mathcal{E}_\lambda^{(-)}\right|}K_0\left(\sqrt{\left|\mathcal{E}_\lambda^{(-)}\right|}\rho\right), |\lambda| < \pi/2,$$

form a complete orthonormalized system in the Hilbert space $L^2(\mathbb{R}_+)$.

Complete Spectrum and Inversion Formulas in Two Dimensions with Pure AB Field

In the previous subsubsections, we have constructed all s.a. radial Hamiltonians associated with the s.a. differential operations $\check{h}(l)$ as s.a. extensions of the symmetric operators $\hat{h}(l)$ for any $l \in \mathbb{Z}$ and for any ϕ_0 and μ. We assemble our previous results into two groups.

For $\mu = 0$, we have the following s.a. radial Hamiltonians:

$$\hat{h}_1(l), \ l \neq l_0, \ D_{h_1(l)} = D^*_{\check{h}(l)}(\mathbb{R}_+),$$

$$\hat{h}_\lambda(l_0), \ \lambda \in \mathbb{S}(-\pi/2, \pi/2), \ D_{h_\lambda(l_0)} \text{ is given by (10.26).}$$

For $\mu > 0$, they are

$$\hat{h}_1(l), \ l \neq l_a = a = 0, -1, \ D_{h_1(l)} = D^*_{\check{h}(l)}(\mathbb{R}_+),$$

$$\hat{h}_{\lambda_a}(l_a), \ \lambda_a \in \mathbb{S}(-\pi/2, \pi/2), \ D_{h_{\lambda_a}(l_a)} \text{ is given by (10.22).}$$

Each set of possible s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(l)$ generates s.a. Hamiltonians in accordance with the relations (10.13) and (10.14). As a final result, we have a family of s.a. rotationally invariant two-dimensional Schrödinger operators $\hat{H}^\perp_{\mathfrak{e}} = M^{-1}\widehat{\mathcal{H}}^\perp_{\mathfrak{e}}$ associated with the s.a. differential operation $\check{H}^\perp$ (10.4) with $B = 0$.

When presenting the spectrum and inversion formulas for $\hat{H}^\perp_{\mathfrak{e}}$, we also consider the cases $\mu = 0$ and $\mu > 0$ separately. We let E denote the spectrum points of $\hat{H}^\perp_{\mathfrak{e}}$ and let Ψ_E denote the corresponding (generalized) eigenfunctions. The spectrum points of the operators $\hat{h}_{\mathfrak{e}}(l)$ and $\hat{H}^\perp_{\mathfrak{e}}$ are evidently related by $\mathcal{E} = ME$. In addition, when writing formulas for eigenfunctions Ψ_E of the operator $\hat{H}^\perp_{\mathfrak{e}}$ in terms of eigenfunctions $U_{\mathcal{E}}$ of the operators $\hat{h}_{\mathfrak{e}}(l)$, we have to introduce the factor $(2\pi\rho)^{-1/2}\,\mathrm{e}^{i\epsilon_q(\phi_0 - l)\varphi}$ in accordance with (10.6) with $\epsilon = \epsilon_q$ (because $\epsilon_B = 1$), to make the substitutions $\mathcal{E} = ME$ and $\mathcal{E}^{(-)}_{\lambda_a} = ME^{(-)}_{\lambda_a}$, $\mathcal{E}^{(-)}_{\lambda} = ME^{(-)}_{\lambda}$ for the respective points of the continuous spectrum and discrete spectrum, and in addition, to multiply eigenfunctions of the continuous spectrum of the operators $\hat{h}_{\mathfrak{e}}(l)$ by the factor $\sqrt{M}$ because of the change of the spectral measure $\mathrm{d}\mathcal{E}$ to the corresponding spectral measure[2] $\mathrm{d}E$.

For $\mu = 0$, there is a family of s.a. two-dimensional Schrödinger operators $\hat{H}^\perp_{\mathfrak{e}} = \hat{H}^\perp_\lambda$ parameterized by a real parameter $\lambda \in \mathbb{S}(-\pi/2, \pi/2)$,

$$\hat{H}^\perp_\lambda = \sum\nolimits^{\oplus}_{l \in \mathbb{Z}, l \neq l_0} \hat{H}^\perp(l) \oplus \hat{H}^\perp_\lambda(l_0),$$

$$\hat{H}^\perp(l) = M^{-1} S_l \hat{h}_{(1)}(l) S_l^{-1}, \ l \neq l_0,$$

$$\hat{H}^\perp_\lambda(l_0) = M^{-1} S_{l_0} \hat{h}_\lambda(l_0) S_{l_0}^{-1}.$$

[2]From a physical standpoint, the latter is related to the change of the "normalization of the eigenfunctions of the continuous spectrum to δ function" from $\delta(\mathcal{E} - \mathcal{E}')$ to $\delta(E - E')$.

The spectrum of $\hat{H}_\lambda^\perp$ is given by

$$\operatorname{spec} \hat{H}_\lambda^\perp = \mathbb{R}_+ \cup \left\{ \begin{array}{l} E_\lambda^{(-)} = -4M^{-1}\kappa_0^2 \exp\left[2(\tan\lambda - \mathbf{C})\right], \ |\lambda| < \pi/2 \\ \varnothing, \ \ \lambda = \pm\pi/2 \end{array} \right\}.$$

The complete system of orthonormalized (generalized) eigenfunctions of $\hat{H}_\lambda^\perp$ consists of the generalized eigenfunctions $\Psi_{l,E}(\rho)$ of the continuous spectrum,

$$\Psi_{l,E}(\rho) = (M/4\pi)^{1/2}\, \mathrm{e}^{i\epsilon_q(\phi_0 - l)\varphi} J_{\varkappa_l}\left(\sqrt{ME}\rho\right), \ \ l \neq l_0\,, \ \ E \geq 0,$$

$$\Psi_{l_0,E}^\lambda(\rho) = \sqrt{\frac{M}{4\pi\left(\tilde{\lambda}^2 + \pi^2/4\right)}}\mathrm{e}^{i\epsilon_q\phi_0\varphi}\left[\tilde{\lambda}J_0\left(\sqrt{ME}\rho\right) + \frac{\pi}{2}N_0(\sqrt{ME}\rho)\right],$$

$$\tilde{\lambda} = \tan\lambda - \mathbf{C} - \ln\left(\sqrt{ME}/2\kappa_0\right),$$

and (in the case of $|\lambda| < \pi/2$) the eigenfunction $\Psi_{l_0}^\lambda(\rho)$ corresponding to the discrete level $E_\lambda^{(-)}$,

$$\Psi_{l_0}^\lambda(\rho) = M\sqrt{\left|E_\lambda^{(-)}\right|/\pi}\,\mathrm{e}^{i\epsilon_q\phi_0\varphi}K_0\left(\sqrt{M\left|E_\lambda^{(-)}\right|}\rho\right),$$

such that

$$\check{H}^\perp\Psi_{l,E}(\rho) = E\Psi_{l,E}(\rho), \ \ \check{H}^\perp\Psi_{l_0,E}^\lambda(\rho) = E\Psi_{l_0,E}^\lambda(\rho), \ \ E \geq 0,$$

$$\hat{H}_\lambda^\perp\Psi_{l_0}^\lambda(\rho) = E_\lambda^{(-)}\Psi_{l_0}^\lambda(\rho), \ \ |\lambda| < \pi/2.$$

The corresponding inversion formulas have the form

$$\begin{aligned}
\Psi(\rho) &= \sum_{l\in\mathbb{Z}, l\neq l_0}\int_0^\infty \Phi_l(E)\Psi_{l,E}(\rho)\mathrm{d}E \\
&\quad + \int_0^\infty \Phi_{l_0}(E)\Psi_{l_0,E}^\lambda(\rho)\mathrm{d}E + \Phi_{l_0}\Psi_{l_0}^\lambda(\rho),
\end{aligned}$$

$$\Phi_l(E) = \int \mathrm{d}\rho\overline{\Psi_{l,E}(\rho)}\Psi(\rho),\ \Phi_{l_0}(E) = \int \mathrm{d}\rho\overline{\Psi_{l_0,E}^\lambda(\rho)}\Psi(\rho),$$

$$\Phi_{l_0} = \int \mathrm{d}\rho\overline{\Psi_{l_0}^\lambda(\rho)}\Psi(\rho),\ \forall\Psi \in L^2\left(\mathbb{R}^2\right),$$

$$\int \mathrm{d}\rho\,|\Psi(\rho)|^2 = \sum_{l\in\mathbb{Z}}\int_0^\infty |\Phi_l(E)|^2\,\mathrm{d}E + |\Phi_{l_0}|^2.$$

The terms with Φ_{l_0} and $\Psi_{l_0}^\lambda(\rho)$ are absent in the case of $|\lambda| = \pi/2$.

For $\mu > 0$, there is a family of s.a. two-dimensional Schrödinger operators $\hat{H}^{\perp}_{\mathfrak{e}} = \hat{H}^{\perp}_{\{\lambda_a\}}$, $a = 0, -1$, parameterized by two real parameters $\lambda_a \in \mathbb{S}(-\pi/2, \pi/2)$,

$$\hat{H}^{\perp}_{\{\lambda_a\}} = \sum_{l \in \mathbb{Z}, l \neq l_a}^{\oplus} \hat{H}^{\perp}(l) \oplus \sum_{a}^{\oplus} \hat{H}^{\perp}_{\lambda_a}(l_a),$$

$$\hat{H}^{\perp}(l) = M^{-1} S_l \hat{h}_{(1)}(l) S_l^{-1},\ l \neq l_a,$$

$$\hat{H}^{\perp}_{\lambda_a}(l_a) = M^{-1} S_{l_a} \hat{h}_{\lambda_a}(l_a) S_{l_a}^{-1}.$$

The spectrum of $\hat{H}^{\perp}_{\{\lambda_a\}}$ is given by

$$\operatorname{spec} \hat{H}^{\perp}_{\{\lambda_a\}} = \mathbb{R}_+ \cup \left\{ \begin{array}{l} E^{(-)}_{\lambda_a} = -4M^{-1}k_0^2 \left|\tilde{\lambda}_a\right|^{-\varkappa_a^{-1}},\ \ \lambda_a \in (-\pi/2, 0) \\ \varnothing,\ \ \lambda_a \notin (-\pi/2, 0) \end{array} \right\},$$

where $\varkappa_a = |\mu + a|$, $\tilde{\lambda}_a = \Gamma(1 - \varkappa_a)\Gamma^{-1}(1 + \varkappa_a)\tan\lambda_a$.

A complete system of orthonormalized (generalized) eigenfunctions of $\hat{H}^{\perp}_{\{\lambda_a\}}$ consists of the generalized eigenfunctions $\Psi_{l,E}(\rho)$, $l \neq l_a$, and $\Psi^{\lambda_a}_{l_a,E}(\rho)$ of the continuous spectrum,

$$\Psi_{l,E}(\rho) = (M/4\pi)^{1/2} \mathrm{e}^{\epsilon_q(\phi_0 - l)\varphi} J_{\varkappa_l}\left(\sqrt{ME}\rho\right),\ \varkappa_l = |l + \mu|,\ l \neq l_a,$$

$$\Psi^{\lambda_a}_{l_a,E}(\rho) = \sqrt{\frac{1}{4\pi Q_a}} \mathrm{e}^{i\epsilon_q(\phi_0 - l_a)\varphi} \left[J_{\varkappa_a}\left(\sqrt{ME}\rho\right) \right.$$
$$\left. + \tilde{\lambda}_a \left(\sqrt{ME}/2\kappa_0\right)^{2\varkappa_a} J_{-\varkappa_a}\left(\sqrt{ME}\rho\right) \right],$$

$$Q_a = 1 + 2\tilde{\lambda}_a (ME/4)^{\varkappa_a} \cos(\pi\varkappa_a) + \left(\tilde{\lambda}_a\right)^2 (ME/4)^{2\varkappa_a},\ E \geq 0,$$

and (in the case of $\lambda_a \in (-\pi/2, 0)$) the eigenfunctions $\Psi^{\lambda_a}_{l_a}(\rho)$ corresponding to the discrete levels $E^{(-)}_{\lambda_a}$,

$$\Psi^{\lambda_a}_{l_a}(\rho) = \sqrt{\frac{M^2 \left|E^{(-)}_{\lambda_a}\right| \sin(\pi\varkappa_a)}{\pi^2 \varkappa_a}} \mathrm{e}^{i\epsilon_q(\phi_0 - l_a)\varphi} K_{\varkappa_a}\left(\sqrt{\left|ME^{(-)}_{\lambda_a}\right|}\rho\right),$$

such that

$$\check{H}^{\perp}\Psi_{l,E}(\rho) = E\Psi_{l,E}(\rho),\ l \neq l_a,\ \ \check{H}^{\perp}\Psi^{\lambda_a}_{l_a,E}(\rho) = E\Psi^{\lambda_a}_{l_a,E}(\rho),\ \ E \geq 0,$$

$$\hat{H}^{\perp}_{\{\lambda_a\}}\Psi^{\lambda_b}_{l_b}(\rho) = E^{(-)}_{\lambda_b}\Psi^{\lambda_b}_{l_b}(\rho),\ \ b = 0, -1.$$

The corresponding inversion formulas have the form

$$\Psi(\rho) = \sum_{l\in\mathbb{Z},\, l\neq l_a} \int_0^\infty \Phi_l(E)\Psi_{l,E}(\rho)\mathrm{d}E + \sum_a \left[\int_0^\infty \Phi_{l_a}(E)\Psi^{\lambda_a}_{l_a,E}(\rho)\mathrm{d}E + \Phi_{l_a}\Psi^{\lambda_a}_{l_a}(\rho)\right],\ \forall\Psi\in L^2\left(\mathbb{R}^2\right),$$

$$\Phi_l(E) = \int \mathrm{d}\rho\overline{\Psi_{l,E}(\rho)}\Psi(\rho),\ l\neq l_a\,,$$

$$\Phi_{l_a}(E) = \int \mathrm{d}\rho\overline{\Psi^{\lambda_a}_{l_a,E}(\rho)}\Psi(\rho),\ \Phi_{l_a} = \int \mathrm{d}\rho\overline{\Psi^{\lambda_a}_{l_a}(\text{æ})}\Psi(\text{æ}),$$

$$\int \mathrm{d}\rho\,|\Psi(\rho)|^2 = \sum_{l\in\mathbb{Z}} \int_0^\infty |\Phi_l(E)|^2\,\mathrm{d}E + \sum_a |\Phi_{l_a}|^2\,.$$

The terms with Φ_{l_a} and $\Psi^{\lambda_a}_{l_a}(\rho)$ are absent in the case of $\lambda_a\notin(-\pi/2,0)$.

We now consider the case of the MSF where $B\neq 0$.

10.2.1.3 Self-adjoint Radial Hamiltonians with MSF

In this case, the radial differential operation $\check{h}(l)$ is given by (10.9) with $\gamma = e|B|/c\hbar\neq 0$,

$$\check{h}(l) = -\partial_\rho^2 + g_1\rho^{-2} + g_2\rho^2 + \mathcal{E}^{(0)}_l,$$
$$g_1 = \varkappa_l^2 - 1/4,\ \varkappa_l = |l+\mu|\,,\ g_2 = \gamma^2/4,\ \mathcal{E}^{(0)}_l = \gamma(l+\mu).$$

Up to the constant term $\mathcal{E}^{(0)}_l$, these s.a. differential operations and the corresponding initial symmetric operators $\hat{h}(l)$ are identical to the respective operations and symmetric operators encountered in Sect. 8.4. We can therefore directly carry over the previously obtained results to s.a. extensions of $\hat{h}(l)$. We note that as in the case of a pure AB field, a division to different regions of g_1 is actually determined by the same term $g_1\rho^{-2}$ singular at the origin and independent of the value of B.

First Region: $g_1\geq 3/4$

In this region, we have $(l+\mu)^2\geq 1$, so that

$$\mu = 0: l\leq -1 \text{ or } l\geq 1,\ \text{i.e., } l\neq l_0\,,$$
$$\mu > 0: l\leq -2 \text{ or } l\geq 1,\ \text{i.e., } l\neq l_a\,.$$

For such l, the initial symmetric operator $\hat{h}(l)$ has zero deficiency indices. It is essentially s.a., and its unique s.a. extension is $\hat{h}_1(l) = \hat{h}^+(l)$ with domain $D^*_{\check{h}(l)}(\mathbb{R}_+)$. The spectrum of $\hat{h}_1(l)$ is simple, discrete, and given by

$$\operatorname{spec}\hat{h}_1(l) = \left\{\mathcal{E}_{l,m} = \gamma\left(1 + |l+\mu| + (l+\mu) + 2m\right),\ m \in \mathbb{Z}_+\right\}. \tag{10.19}$$

The eigenfunctions $U^{(1)}_{l,m}$,

$$\begin{aligned} U^{(1)}_{l,m}(\rho) &= Q_{l,m}\,(\gamma/2)^{1/4+\varkappa_l/2}\,\rho^{1/2+\varkappa_l}\,\mathrm{e}^{-\gamma\rho^2/4}\Phi\left(-m, 1+\varkappa_l; \gamma\rho^2/2\right), \\ Q_{l,m} &= \left(\frac{\sqrt{2\gamma}\,\Gamma(1+\varkappa_l+m)}{m!\,\Gamma^2(1+\varkappa_l)}\right)^{1/2}, \end{aligned} \tag{10.20}$$

of the Hamiltonian $\hat{h}_1(l)$ form a complete orthonormalized system in the Hilbert space $L^2(\mathbb{R}_+)$.

Second Region: $-1/4 < g_1 < 3/4$

In this region, we have $0 < (l+\mu)^2 < 1$, or equivalently (10.15). We know that if $\mu = 0$, these inequalities have no solutions for $l \in \mathbb{Z}$, while if $\mu > 0$ there are the two solutions $l = l_a = a$, $a = 0, -1$. Therefore, we again remain with the case $\mu > 0$.

For each $l = l_a$, there exists a one-parameter $U(1)$ family of s.a. radial Hamiltonians $\hat{h}_{\lambda_a}(l_a)$ parameterized by a real parameter $\lambda_a \in \mathbb{S}(-\pi/2, \pi/2)$. These Hamiltonians are specified by the asymptotic s.a. boundary conditions at $\rho \to 0$,

$$\psi_{\lambda_a}(\rho) = C\left[\left(\sqrt{\gamma/2}\rho\right)^{1/2+\varkappa_a}\sin\lambda_a + \left(\sqrt{\gamma/2}\rho\right)^{1/2-\varkappa_a}\cos\lambda_a\right] + O\left(\rho^{3/2}\right), \tag{10.21}$$

where $\varkappa_a = |\mu + a|, 0 < \varkappa_a < 1$, and C is an arbitrary constant,[3] and their domains are given by

$$D_{h_{\lambda_a}(l_a)} = \left\{\psi : \psi \in D^*_{\check{h}(l_a)}(\mathbb{R}_+),\ \psi \text{ satisfy (10.21)}\right\}. \tag{10.22}$$

The spectrum of $\hat{h}_{\lambda_a}(l_a)$ is simple, discrete, and is bounded from below,

$$\operatorname{spec}\hat{h}_{\lambda_a}(l_a) = \left\{\mathcal{E}_{a,m} = \tau_{a,m} + \mathcal{E}^{(0)}_{l_a},\ m \in \mathbb{Z}_+\right\},$$

[3] In comparison with (10.16), we fix the dimensional parameter k_0 by $k_0 = \sqrt{\gamma/2}$.

where $\tau_{a,m}$ are solutions of the equation $\omega_{\lambda_a}(\tau_{a,m}) = 0$,

$$\omega_{\lambda_a}(W) = \omega_+(W)\sin\lambda_a + \omega_-(W)\cos\lambda_a,$$
$$\omega_\pm(W) = \Gamma(1 \pm \varkappa_a)/\Gamma(1/2 \pm \varkappa_a/2 - W/2\gamma). \quad (10.23)$$

The eigenfunctions $U^{(2)}_{\lambda_a,m}$,

$$U^{(2)}_{\lambda_a,m}(\rho) = Q_{a,m}\left[u_+(\rho;\tau_{a,m})\sin\lambda_a + u_-(\rho;\tau_{a,m})\cos\lambda_a\right],$$
$$Q_{a,m} = \left(\frac{\tilde{\omega}_{\lambda_a}(\tau_{a,m})}{\sqrt{2\gamma}\varkappa_a\omega'_{\lambda_a}(\tau_{a,m})}\right)^{1/2},$$
$$\tilde{\omega}_{\lambda_a}(W) = \omega_+(W)\cos\lambda_a - \omega_-(W)\sin\lambda_a,$$
$$u_\pm(\rho;W) = (\gamma/2)^{1/4\pm\varkappa_a/2}\rho^{1/2\pm\varkappa_a}e^{-\gamma\rho^2/4}\Phi\left(1/2 \pm \varkappa_a/2 - W/2\gamma, 1 \pm \varkappa_a; \gamma\rho^2/2\right), \quad (10.24)$$

of the Hamiltonian $\hat{h}_{\lambda_a}(l_a)$ form a complete orthonormalized system in the Hilbert space $L^2(\mathbb{R}_+)$.

For $\lambda_a = \pm\pi/2$ and $\lambda_a = 0$ one can easily obtain explicit expressions for the spectrum and eigenfunctions. For $\lambda_a = \pm\pi/2$, they are given by the respective formulas (10.19) and (10.20) with the substitutions $l \to l_a$ and $\varkappa_l \to \varkappa_a$. For $\lambda_a = 0$, these formulas are modified by the additional substitution $\varkappa_a \to -\varkappa_a$. In addition, one can see that in each interval $\left(\tau^{(\pm\pi/2)}_{a,m}, \tau^{(\pm\pi/2)}_{a,m+1}\right)$, $m \in \{-1\} \cup \mathbb{Z}_+$, where $\tau^{(\pm\pi/2)}_{a,m}$, $m \in \mathbb{Z}_+$, are solutions of the equation $\omega_{\pm\pi/2}(\tau_{a,m}) = 0$, and we set formally $\tau^{(\pm\pi/2)}_{a,-1} = -\infty$. There is one solution $\tau_{a,m}$ of the equation $\omega_{\lambda_a}(\tau_{a,m}) = 0$ for a fixed $\lambda_a \in (-\pi/2, \pi/2)$; the solution $\tau_{a,m}$ increases monotonically from $\tau^{(\pm\pi/2)}_{a,m} + 0$ to $\tau^{(\pm\pi/2)}_{a,m+1} - 0$ as λ_a goes from $-\pi/2 + 0$ to $\pi/2 - 0$.

Third Region: $g_1 = -1/4$

In this region, we have $l + \mu = 0$. Thus, we remain with the only case, $\mu = 0$, and with $l = l_0 = 0$.

For $l = l_0$, there exists a one-parameter $U(1)$ family of s.a. radial Hamiltonians $\hat{h}_\lambda(l_0)$, parameterized by the real parameter $\lambda \in \mathbb{S}(-\pi/2, \pi/2)$. These Hamiltonians are specified by the asymptotic s.a. boundary conditions at $\rho \to 0$,

$$\psi_\lambda(\rho) = C\left[\rho^{1/2}\ln\left(\sqrt{\gamma/2}\rho\right)\cos\lambda + \rho^{1/2}\sin\lambda\right] + O\left(\rho^{3/2}\ln\rho\right), \quad (10.25)$$

where C is an arbitrary constant, and their domains are given by

$$D_{h_\lambda(l_0)} = \left\{\psi : \psi \in D^*_{\check{h}(l_0)}(\mathbb{R}_+), \ \psi \text{ satisfy } (10.25)\right\}. \tag{10.26}$$

The spectrum of $\hat{h}_\lambda(l_0)$ is simple, discrete, and is bounded from below, and

$$\operatorname{spec} \hat{h}_\lambda(l_0) = \left\{\mathcal{E}_m, \ m \in \left\{\begin{array}{l} \mathbb{Z}_+, \ \lambda = \pm\pi/2 \\ \{-1\} \cup \mathbb{Z}_+, \ |\lambda| < \pi/2 \end{array}\right.\right\},$$

where $\mathcal{E}_m$ are solutions of the equation $\omega_\lambda(\mathcal{E}_m) = 0$,

$$\omega_\lambda(W) = \cos\lambda[\psi(\alpha_0) - 2\psi(1)] - \sin\lambda, \ \ \alpha_0 = 1/2 - W/2\gamma. \tag{10.27}$$

The limit $\lambda \to \pm\pi/2$ in this equation and its solutions is described by the equation $\psi^{-1}(\alpha_0) = 0$ or $1/2 - \mathcal{E}_m^{(\pm\pi/2)}/2\gamma = -m$, $m \in \mathbb{Z}_+$, and by the solution $\mathcal{E}_m^{(\pm\pi/2)} = \gamma(1+2m)$.

A qualitative description of the spectrum is given in Sect. 8.4. One can see that in each interval $\left(\mathcal{E}_m^{(\pm\pi/2)}, \mathcal{E}_{m+1}^{(\pm\pi/2)}\right)$, $m \in \{-1\} \cup \mathbb{Z}_+$, there is one solution $\mathcal{E}_m$ (for a fixed $\lambda \in (-\pi/2, \pi/2)$) of (10.27) (we set formally $E_{-1}^{(\pm\pi/2)} = -\infty$); the solution $\mathcal{E}_m$ increases monotonically from $\mathcal{E}_m^{(\pm\pi/2)} + 0$ to $\mathcal{E}_{m+1}^{(\pm\pi/2)} - 0$ as λ goes from $\pi/2 - 0$ to $-\pi/2 + 0$.

The eigenfunctions $U^{(3)}_{\lambda,m}$,

$$\begin{aligned}
U^{(3)}_{\lambda,m} &= Q_{\lambda,m}\left[u_1(\rho;\mathcal{E}_m)\sin\lambda + u_3(\rho;\mathcal{E}_m)\cos\lambda\right], \\
u_1(\rho;W) &= (\gamma/2)^{1/4}\rho^{1/2}\mathrm{e}^{-\gamma\rho^2/4}\Phi\left(\alpha_0, 1; \gamma\rho^2/2\right), \\
u_3(\rho;W) &= u_1(\rho;W)\ln\left(\sqrt{\gamma/2}\rho\right) \\
&\quad + (\gamma/2)^{1/4}\rho^{1/2}\mathrm{e}^{-\gamma\rho^2/4}\,\partial_\mu\Phi(1/2+\mu-W/2\gamma, 1+2\mu; \gamma\rho^2/2)\big|_{\mu=0}, \\
Q_{\lambda,m} &= \left[-\frac{\tilde{\omega}_\lambda(\mathcal{E}_m)}{\sqrt{2\gamma}\,\omega'_\lambda(\mathcal{E}_m)}\right]^{1/2}, \ \tilde{\omega}_\lambda(W) = \sin\lambda[\psi(\alpha_0) - 2\psi(1)] + \cos\lambda,
\end{aligned} \tag{10.28}$$

of the Hamiltonians $\hat{h}_\lambda(l_0)$, form a complete orthonormalized system in the Hilbert space $L^2(\mathbb{R}_+)$.

We note that the spectrum and eigenfunctions in the case $\lambda = \pm\pi/2$ can be obtained from the respective formulas for the first region in the formal limit $l \to 0$.

10.2.1.4 Complete Spectrum and Inversion Formulas in Two Dimensions with MSF

In the previous subsubsections, we constructed all s.a. radial Hamiltonians associated with the s.a. differential operation $\check{h}(l)$ as s.a. extensions of the symmetric operator $\hat{h}(l)$ for any $l \in \mathbb{Z}$ and for any ϕ_0, μ, and B. We assemble our previous results into two groups.

For $\mu = 0$, we have

$$\hat{h}_1(l), \;\; l \neq l_0 = 0, \;\; D_{h_1(l)} = D^*_{\check{h}(l)}(\mathbb{R}_+),$$
$$\hat{h}_\lambda(l_0), \;\; \lambda \in \mathbb{S}(-\pi/2, \pi/2),$$

and the domain $D_{h_\lambda(l_0)}$ is given by (10.26).

For $\mu > 0$, we have

$$\hat{h}_1(l), \;\; l \neq l_a = a = 0, -1, \;\; D_{h_1(l)} = D^*_{\check{h}(l)}(\mathbb{R}_+),$$
$$\hat{h}_{\lambda_a}(l_a), \;\; \lambda_a \in \mathbb{S}(-\pi/2, \pi/2),$$

and the domain $D_{h_{\lambda_a}(l_a)}$ is given by (10.22).

As a result, each set of possible s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(l)$ generates an s.a. rotationally invariant Schrödinger operator $\hat{H}^{\perp}_{\mathfrak{e}} = M^{-1}\widehat{\mathcal{H}}^{\perp}_{\mathfrak{e}}$ in accordance with relations (10.13) and (10.14). As in the case of a pure AB field where $B = 0$, we let E denote the spectrum points of $\hat{H}^{\perp}_{\mathfrak{e}}$.

It is convenient to change the indexing l, m of the spectrum points and eigenfunctions to l, n, as follows:

$$n = n(l,m) = \begin{cases} m, \; l \leq -1, \\ m + l, \; l \geq 0, \end{cases} \qquad m \in \mathbb{Z}_+, \; l \in \mathbb{Z};$$
$$m = m(n,l) = \begin{cases} n, \; l \leq -1, \\ n - l, \; 0 \leq l \leq n, \end{cases} \qquad n \in \mathbb{Z}_+, \; l \in \mathbb{Z}, \tag{10.29}$$

and then to interchange their positions, so that finally, the indices l, m are replaced by indices n, l.

When writing formulas for eigenfunctions $\Psi_{n,l}$ of an operator $\hat{H}^{\perp}_{\mathfrak{e}}$ in terms of eigenfunctions $U_{l,m}$ of the operators $\hat{h}_{\mathfrak{e}}(l)$, we have to introduce the factor $(2\pi\rho)^{-1/2}\,\mathrm{e}^{i\epsilon(\phi_0 - l)\varphi}$ in accordance with (10.6) and to make the substitution $\mathcal{E}_{l,m} = ME_{n,l}$ for the corresponding spectrum points.

The final result is the following. There is a family of s.a. two-dimensional Schrödinger operators $\hat{H}^{\perp}_{\mathfrak{e}}$ parameterized by real parameters λ_*, such that $\hat{H}^{\perp}_{\mathfrak{e}} = \hat{H}^{\perp}_{\lambda_*}$,

$$\hat{H}_{\lambda_*}^{\perp} = \sum\nolimits_{l\in\mathbb{Z},l\neq l_*}^{\oplus} \hat{H}^{\perp}(l) \oplus \sum\nolimits_{l_*}^{\oplus} \hat{H}_{\lambda_*}^{\perp}(l_*),$$
$$\hat{H}^{\perp}(l) = M^{-1}S_l\hat{h}_1(l)S_l^{-1},\ l\neq l_*,$$
$$\hat{H}_{\lambda_*}^{\perp}(l_*) = M^{-1}S_{l_*}\hat{h}_{\lambda_*}(l_*)S_{l_*}^{-1},$$
$$l_* = \begin{cases} l_0,\ \mu=0, \\ l_a,\ \mu>0, \end{cases} \quad \lambda_* = \begin{cases} \lambda\in\mathbb{S}(-\pi/2,\pi/2),\ \mu=0, \\ \lambda_a\in\mathbb{S}(-\pi/2,\pi/2),\ \mu>0. \end{cases} \tag{10.30}$$

The spectrum of $\hat{H}_{\lambda_*}^{\perp}$ is given by

$$\text{spec }\hat{H}_{\lambda_*}^{\perp} = \left\{\cup_{l\in\mathbb{Z},l\neq l_*}(E_{n,l},\ n\in\mathbb{Z}_+)\right\}\cup\left\{\cup_{l=l_*}\left(E_n^{(\lambda_*)},\ n\in\mathbb{Z}_+\right)\right\},$$
$$E_{n,l} = \gamma M^{-1}[1+2n+2\theta(l)\mu],\ l\leq n,\ l\neq l_*,\ \theta(l) = \begin{cases} 1,\ l\geq 0, \\ 0,\ l<0, \end{cases} \tag{10.31}$$

$$E_n^{(\lambda)}: \begin{cases} \omega_\lambda\left(ME_n^{(\lambda)}\right)=0,\ |\lambda|<\pi/2, \\ E_n^{(\pm\pi/2)} = \gamma M^{-1}(1+2n), \end{cases} \quad \mu=0,$$
$$\begin{cases} E_n^{(\lambda_a)} = M^{-1}[\tau_{a,n}+\gamma(a+\mu)],\ \omega_{\lambda_a}(\tau_{a,n})=0, \\ E_n^{(\pm\pi/2)} = \gamma M^{-1}[1+2n+2\theta(a)\mu], \end{cases} \quad n\in\mathbb{Z}_+,\mu>0, \tag{10.32}$$

where $\omega_\lambda(W)$ and $\omega_{\lambda_a}(W)$ are given respectively by (10.27) and (10.23).

A complete set of orthonormalized eigenfunctions of $\hat{H}_{\lambda_*}^{\perp}$ consists of the functions $\Psi_{n,l}(\rho),\ l\neq l_*$, and $\Psi_{n,l_*}^{\lambda_*}(\rho)$,

$$\Psi_{n,l}(\boldsymbol{æ}) = \frac{1}{\sqrt{2\pi\rho}}\mathrm{e}^{i\epsilon(\phi_0-l)\varphi}U_{l,m(n,l)}^{(1)}(\rho), \tag{10.33}$$

where $U_{l,m}^{(1)}(\rho)$ are given by (10.20), and (we note that $m(n,l_*)=n$)

$$\Psi_{n,l_0}^{\lambda}(\rho) = \frac{1}{\sqrt{2\pi\rho}}\mathrm{e}^{i\epsilon\phi_0\varphi}U_{\lambda,n}^{(3)}(\rho),\ \mu=0,$$
$$\Psi_{n,l_a}^{\lambda_a}(\rho) = \frac{1}{\sqrt{2\pi\rho}}\mathrm{e}^{i\epsilon(\phi_0-l_a)\varphi}U_{\lambda_a,n}^{(2)}(\rho),\ \mu>0,$$

where $U_{\lambda,n}^{(3)}(\rho)$ and $U_{\lambda_a,n}^{(2)}(\rho)$ are given respectively by (10.28) and (10.24), so that

$$\hat{H}_{\lambda_*}^{\perp}\Psi_{n,l}(\rho) = E_{n,l}\Psi_{n,l}(\rho),\ l\neq l_*,\ \ \hat{H}_{\lambda_*}^{\perp}(\rho)\Psi_{n,l_*}^{\lambda_*} = E_n^{(\lambda_*)}\Psi_{n,l_*}^{\lambda_*}(\rho).$$

We note that for the case of $\lambda = \pm\pi/2$, $l = l_0 = 0$, and for the case of $\lambda_a = \pm\pi/2$, $l = l_a = a = 0, -1$, the energy eigenvalues $E_n^{(\lambda)}$ and $E_n^{(\lambda_a)}$ and the corresponding eigenfunctions Ψ_n^{λ} and $\Psi_n^{\lambda_a}$ are given respectively by (10.31) and (10.33) extended to all values of l.

The corresponding inversion formulas have the form

$$\Psi(\rho) = \sum_{l\in\mathbb{Z},\ l\neq l_*}\sum_{n\in\mathbb{Z}_+}\Phi_{n,l}\Psi_{n,l}(\rho) + \sum_{l_*,n\in\mathbb{Z}_+}\Phi_{n,l_*}\Psi_{n,l_*}^{\lambda_*}(\rho),$$

$$\Phi_{n,l} = \int d\rho\overline{\Psi_{n,l}(\rho)}\Psi(\rho),\ l\neq l_*,\ \Phi_{n,l_*} = \int d\rho\overline{\Psi_{n,l_*}^{\lambda_*}(\rho)}\Psi(\rho),$$

$$\int d\rho\,|\Psi(\rho)|^2 = \sum_{l\in\mathbb{Z}}\sum_{n\in\mathbb{Z}_+}|\Phi_{n,l}|^2,\ \forall\Psi\in L^2\left(\mathbb{R}^2\right).$$

10.2.2 Three-Dimensional Case

In three dimensions, we start with the differential operation $\check{H}$ (10.3). The initial symmetric operator $\hat{H}$ associated with $\check{H}$ is defined on the domain $D_H = \mathcal{D}\left(\mathbb{R}^3\setminus\mathbb{R}_z\right) \in \mathfrak{H} = L^2(\mathbb{R}^3)$, where $\mathcal{D}\left(\mathbb{R}^3\setminus\mathbb{R}_z\right)$ is the space of smooth and compactly supported functions vanishing in a neighborhood of the z-axis. The domain D_H is dense in $\mathfrak{H}$, and the symmetry of $\hat{H}$ is obvious. An s.a. Schrödinger operator must be defined as an s.a. extension of $\hat{H}$.

There is an evident spatial symmetry in the classical description of the system, the symmetry with respect to rotations around the z-axis and translations along this axis, which is manifested as the invariance of the classical Hamiltonian under these space transformations. The key point in constructing a quantum description of the system is the requirement of the invariance of the Schrödinger operator under the same transformations. Namely, let $\mathbb{G}$ be the group of the above space transformations S : $\mathbf{r} \longmapsto S\mathbf{r}$. This group is unitarily represented in $\mathfrak{H}$: if $S \in \mathbb{G}$, then the corresponding operator U_S is defined by

$$(U_S\psi)(\mathbf{r}) = \psi\left(S^{-1}\mathbf{r}\right),\ \forall\psi\in\mathfrak{H}.$$

The operator $\hat{H}$ evidently commutes[4] with U_S for any S.

We search only for s.a. extensions $\hat{H}_{\mathfrak{e}}$ of $\hat{H}$ that also commute with U_S for any S. This condition is the explicit form of the invariance, or symmetry, of a Schrödinger operator under the space transformations. As in classical mechanics,

[4]We remind the reader of the notion of commutativity in this case (where one of the operators, U_S, is bounded and defined everywhere): we say that the operators $\hat{H}$ and U_S commute if $U_S\hat{H} \subseteq \hat{H}U_S$, that is, if $\psi\in D_H$, then also $U_S\psi\in D_H$ and $U_S\hat{H}\psi = \hat{H}U_S\psi$.

this symmetry allows for the separation of the cylindrical coordinates ρ, φ, and z and the reduction of the three-dimensional problem to a one-dimensional radial problem. Let $L^2(\mathbb{R}\times\mathbb{R}_+)$ denote the space of square-integrable functions with respect to the Lebesgue measure $\mathrm{d}p_z\mathrm{d}\rho$ on $\mathbb{R}\times\mathbb{R}_+$, and let $V\colon \sum_{l\in\mathbb{Z}}^{\oplus} L^2(\mathbb{R}\times\mathbb{R}_+) \longmapsto \mathfrak{H}$ be the unitary operator defined by the relationship

$$(Vf)(\rho,\varphi,z) = \frac{1}{2\pi\sqrt{\rho}}\int_{\mathbb{R}_z}\mathrm{d}p_z\sum_{l\in\mathbb{Z}}\mathrm{e}^{i(\epsilon(\phi_0-l)\varphi+p_z z)}f(l,p_z,\rho).$$

Similarly to the preceding subsection, it is natural to expect that any s.a. Schrödinger operator $\hat{H}_{\mathfrak{e}}$ can be represented in a form of the type

$$\hat{H}_{\mathfrak{e}}=V\int_{\mathbb{R}_z}\mathrm{d}p_z\sum_{l\in\mathbb{Z}}\hat{h}_{\mathfrak{e}}(l,p_z)V^{-1},$$

where $\hat{h}_{\mathfrak{e}}(l,p_z)$ for fixed l and p_z is an s.a. extension of the symmetric operator $\hat{h}(l,p_z)=\hat{h}(l)+p_z^2/2m_e$ in $L^2(\mathbb{R}_+)$ and the operator $\hat{h}(l)$ in $L^2(\mathbb{R}_+)$ is defined on the domain $D_{h(l)}=\mathcal{D}(\mathbb{R}_+)$, where it acts as

$$\check{h}(l)=-\partial_\rho^2+\rho^{-2}\left[\left(l+\mu+\gamma\rho^2/2\right)^2-1/4\right].$$

The correct expression for $\hat{H}_{\mathfrak{e}}$ can be written in terms of a suitable direct integral,

$$\hat{H}_{\mathfrak{e}}=V\int_{\mathbb{R}_z}^{\oplus}\mathrm{d}p_z\sum_{l\in\mathbb{Z}}^{\oplus}\hat{h}_{\mathfrak{e}}(l,p_z)\,V^{-1}.$$

Its rigorous justification is discussed in [78].

The inversion formulas in three dimensions are obtained by the following modifications in the two-dimensional inversion formulas: $\sum_{l\in\mathbb{Z}}\int\mathrm{d}E \rightarrow \int\mathrm{d}p_z\sum_{l\in\mathbb{Z}}\int\mathrm{d}E^{\perp}$, where $E^{\perp}$ are spectrum points of two-dimensional s.a. Schrödinger operators $\hat{H}_{\mathfrak{e}}^{\perp}$, whereas the eigenvalues (spectrum points) E of three-dimensional s.a. Schrödinger operators $\hat{H}_{\mathfrak{e}}$ are $E=E^{\perp}+p_z^2/2m$, $p_z\in\mathbb{R}$.

(1) The contributions of discrete spectrum points of the two-dimensional s.a. Schrödinger operator $\hat{H}_{\mathfrak{e}}^{\perp}$ have to be multiplied by $\int\mathrm{d}p_z$.
(2) Eigenfunctions of two-dimensional s.a. Schrödinger operators $\hat{H}_{\mathfrak{e}}^{\perp}$ have to be multiplied by $(2\pi\hbar)^{-1/2}\,\mathrm{e}^{ip_z z/\hbar}$ in order to obtain eigenfunctions of three-dimensional s.a. Schrödinger operators $\hat{H}_{\mathfrak{e}}$.
(3) The extension parameters λ_a and λ have to be replaced by functions $\lambda_a(p_z)$ and $\lambda(p_z)$.

10.2.2.1 Self-adjoint Schrödinger Operators with AB Field

For the case of $\mu = 0$, there is a family of s.a. three-dimensional Schrödinger operators parameterized by a real-valued function $\lambda(p_z) \in \mathbb{S}(-\pi/2, \pi/2)$, $p_z \in \mathbb{R}$.

The spectrum of $\hat{H}_{\lambda(p_z)}$ is given by

$$\begin{aligned}
&\operatorname{spec} \hat{H}_{\{\lambda(p_z)\}} \\
&\quad = \mathbb{R}_+ \cup \left\{ \begin{array}{l} p_z^2/2m_e - 4M^{-1}\kappa_0^2 \exp\left[2(\tan\lambda(p_z) - \mathbf{C})\right], \ |\lambda(p_z)| < \pi/2 \\ \varnothing, \ \ \lambda(p_z) = \pm\pi/2 \end{array} \right\}.
\end{aligned}$$

A complete system of orthonormalized generalized eigenfunctions of $\hat{H}_{\lambda(p_z)}$ consists of functions $\Psi_{l,p_z,E^\perp}(\mathbf{r})$, $l \neq l_0$, and $\Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r})$,

$$\begin{aligned}
\Psi_{l,p_z,E^\perp}(\mathbf{r}) &= \left(8\pi^2\hbar/M\right)^{-1/2} \mathrm{e}^{ip_z z/\hbar + i\epsilon_q(\phi_0 - l)\varphi} J_{\varkappa_l}\left(\sqrt{ME^\perp}\rho\right), \\
\Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r}) &= \left(8\pi^2\hbar\left(\tilde{\lambda}^2 + \pi^2/4\right)\Big/ M\right)^{-1/2} \mathrm{e}^{ip_z z/\hbar + i\epsilon_q\phi_0\varphi} \\
&\quad \times \left[\tilde{\lambda} J_0\left(\sqrt{ME^\perp}\rho\right) + \frac{\pi}{2} N_0\left(\sqrt{ME^\perp}\rho\right)\right], \\
\tilde{\lambda} &= \tan\lambda(p_z) - \mathbf{C} - \ln\left(\sqrt{ME^\perp}/2\kappa_0\right),
\end{aligned}$$

and functions $\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r})$,

$$\begin{aligned}
\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r}) &= \frac{1}{2\pi\sqrt{\hbar}} \mathrm{e}^{ip_z z/\hbar + i\epsilon_q\phi_0\varphi} \\
&\quad \times \left\{ \begin{array}{l} \sqrt{2M^2\left|E^{\perp(-)}_{\lambda(p_z)}\right|} K_0\left(\sqrt{M\left|E^{\perp(-)}_{\lambda(p_z)}\right|}\rho\right), \ |\lambda(p_z)| < \pi/2 \\ 0, \ \ \lambda(p_z) = \pm\pi/2 \end{array} \right., \\
E^{\perp(-)}_{\lambda(p_z)} &= -4M^{-1}\kappa_0^2 \exp 2(\tan\lambda(p_z) - \mathbf{C}),
\end{aligned}$$

such that

$$\begin{aligned}
\check{H}\Psi_{l,p_z,E^\perp}(\mathbf{r}) &= \left(p_z^2/2m_e + E^\perp\right)\Psi_{l,p_z,E^\perp}(\mathbf{r}), \ E^\perp \geq 0, \\
\check{H}\Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r}) &= \left(p_z^2/2m_e + E^\perp\right)\Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r}), \ E^\perp \geq 0, \\
\check{H}\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r}) &= \left(p_z^2/2m_e + E^{\perp(-)}_{\lambda(p_z)}\right)\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r}).
\end{aligned}$$

The corresponding inversion formulas have the form

$$\Psi(\mathbf{r}) = \int \mathrm{d}p_z \left[\sum_{l\in\mathbb{Z},\, l\neq 0} \int_0^\infty \Phi_{l,p_z}\left(E^\perp\right) \Psi_{l,p_z,E^\perp}(\mathbf{r})\mathrm{d}E^\perp \right.$$

$$\left. + \int_0^\infty \Phi_{l_0,p_z}\left(E^\perp\right) \Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r})\mathrm{d}E^\perp + \Phi_{l_0,p_z}\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r}) \right],$$

$$\forall \Psi \in L^2\left(\mathbb{R}^3\right),$$

$$\Phi_{l,p_z}\left(E^\perp\right) = \int \overline{\Psi_{l,p_z,E^\perp}(\mathbf{r})}\Psi(\mathbf{r})\mathrm{d}\mathbf{r},\; l \neq l_0,$$

$$\Phi_{l,p_z}\left(E^\perp\right) = \int \overline{\Psi^{\lambda(p_z)}_{l_0,p_z,E^\perp}(\mathbf{r})}\Psi(\mathbf{r})\mathrm{d}\mathbf{r},\; \Phi_{l_0,p_z} = \int \overline{\Psi^{\lambda(p_z)}_{l_0,p_z}(\mathbf{r})}\Psi(\mathbf{r})\mathrm{d}\mathbf{r},$$

$$\int |\Psi(\mathbf{r})|^2\,\mathrm{d}\mathbf{r} = \int \mathrm{d}p_z \left[\sum_{l\in\mathbb{Z}} \int_0^\infty \left|\Phi_{l,p_z}\left(E^\perp\right)\right|^2 \mathrm{d}E^\perp + \left|\Phi_{l_0,p_z}\right|^2 \right].$$

In the case $\mu > 0$, there is a family of s.a. three-dimensional Hamiltonians $\hat{H}_{\{\lambda_a(p_z)\}}$ parameterized by two real-valued functions $\lambda_a(p_z) \in \mathbb{S}(-\pi/2, \pi/2)$, $a = 0, -1$, $p_z \in \mathbb{R}$.

The spectrum of $\hat{H}_{\{\lambda_a(p_z)\}}$ is given by

$$\mathrm{spec}\,\hat{H}_{\{\lambda_a(p_z)\}} = \left\{ \begin{array}{l} p_z^2/2m_e - 4M^{-1}k_0^2 \left|\tilde{\lambda}_a\right|^{-\varkappa_a^{-1}},\; \lambda_a(p_z) \in (-\pi/2, 0) \\ \varnothing,\; \lambda_a(p_z) \notin (-\pi/2, 0) \end{array} \right\} \cup \mathbb{R}_+,$$

$$\varkappa_a = |\mu + a|,\; \tilde{\lambda}_a = \Gamma(1-\varkappa_a)\Gamma^{-1}(1+\varkappa_a)\tan\lambda_a(p_z),\; \varkappa_a = |\mu + a|.$$

A complete orthonormalized system in $L^2\left(\mathbb{R}^3\right)$ consists of both generalized eigenfunctions $\Psi_{l,p_z,E^\perp}(\mathbf{r}), l \neq l_a$, and $\Psi^{\lambda_a(p_z)}_{l_a,p_z,E^\perp}(\mathbf{r})$,

$$\Psi_{l,p_z,E^\perp}(\mathbf{r}) = \left(8\pi^2\hbar/M\right)^{-1/2} \mathrm{e}^{ip_z z/\hbar + i\epsilon_q(\phi_0 - l)\varphi} J_{\varkappa_l}\left(\sqrt{ME^\perp}\rho\right),$$

$$\Psi^{\lambda_a(p_z)}_{l_a,p_z,E^\perp}(\mathbf{r}) = \left(8\pi^2\hbar Q_a\right)^{-1/2} \mathrm{e}^{ip_z z/\hbar + i\epsilon_q(\phi_0 - l_a)\varphi}$$

$$\times \left[J_{\varkappa_a}\left(\sqrt{ME^\perp}\rho\right) + \left(\sqrt{ME^\perp}\Big/ 2\kappa_0\right)^{2\varkappa_a} \tilde{\lambda}_a\, J_{-\varkappa_a}\left(\sqrt{ME^\perp}\rho\right) \right],$$

$$Q_a = 1 + 2\left(ME^\perp/4\right)^{\varkappa_a} \tilde{\lambda}_a \cos(\pi\varkappa_a) + (ME/4)^{2\varkappa_a}\tilde{\lambda}_a^2,$$

and eigenfunctions $\Psi^{\lambda_a(p_z)}_{l_a,p_z}(\mathbf{r})$,

$$\Psi_{l_a,p_z}^{\lambda_a(p_z)}(\mathbf{r}) = \left(2\pi^2\hbar\right)^{-1} \mathrm{e}^{ip_z z/\hbar + i(l_a+\epsilon_q\phi_0)\varphi}$$
$$\times \begin{cases} \sqrt{\frac{M^2\left|E_{\lambda_a(p_z)}^{\perp(-)}\right|\sin(\pi\varkappa_a)}{2\pi\varkappa_a}} K_{\varkappa_a}\left(\sqrt{M\left|E_{\lambda_a(p_z)}^{\perp(-)}\right|}\rho\right), \lambda_a(p_z) \in (-\pi/2, 0) \\ 0,\ \lambda_a(p_z) \notin (-\pi/2, 0) \end{cases},$$
$$E_{\lambda_a(p_z)}^{\perp(-)} = -4M^{-1}\kappa_0^2 \exp 2(\tan\lambda_a(p_z) - \mathbf{C}),$$

such that

$$\check{H}\Psi_{l,p_z,E^\perp}(\mathbf{r}) = \left(p_z^2/2m_e + E^\perp\right)\Psi_{l,p_z,E^\perp}(\mathbf{r}),\ E^\perp \geq 0,$$
$$\check{H}\Psi_{l_a,p_z,E^\perp}^{\lambda_a(p_z)}(\mathbf{r}) = \left(p_z^2/2m_e + E^\perp\right)\Psi_{l_a,p_z,E^\perp}^{\lambda_a(p_z)}(\mathbf{r}),\ E^\perp \geq 0,$$
$$\check{H}\Psi_{l_a,p_z}^{\lambda_a(p_z)}(\mathbf{r}) = \left(p_z^2/2m_e + E_{\lambda_a(p_z)}^{\perp(-)}\right)\Psi_{l_a,p_z}^{\lambda_a(p_z)}(\mathbf{r}).$$

The corresponding inversion formulas have the form

$$\Psi(\mathbf{r}) = \int \mathrm{d}p_z \left[\sum_{l\in\mathbb{Z},\ l\neq l_a} \int_0^\infty \Phi_{l,p_z}\left(E^\perp\right)\Psi_{l,p_z,E^\perp}(\mathbf{r})\mathrm{d}E^\perp \right.$$
$$\left. + \sum_a \int_0^\infty \Phi_{l_a,p_z}\left(E^\perp\right)\Psi_{l_a,p_z,E^\perp}^{\lambda_a(p_z)}(\mathbf{r})\mathrm{d}E^\perp + \Phi_{l_a,p_z}\Psi_{l_a,p_z}^{\lambda_a(p_z)}(\mathbf{r})\right],$$
$$\forall\Psi \in L^2\left(\mathbb{R}^3\right),$$
$$\Phi_{l,p_z}\left(E^\perp\right) = \int \mathrm{d}\mathbf{r}\overline{\Psi_{l,p_z,E^\perp}(\mathbf{r})}\Psi(\mathbf{r}),\ E^\perp \geq 0,\ l \neq l_a,$$
$$\Phi_{l_a,p_z}\left(E^\perp\right) = \int \mathrm{d}\mathbf{r}\overline{\Psi_{l_a,p_z,E^\perp}^{\lambda_a(p_z)}(\mathbf{r})}\Psi(\mathbf{r}),\ E^\perp \geq 0,$$
$$\Phi_{l_a,p_z} = \int \mathrm{d}\mathbf{r}\overline{\Psi_{l_a,p_z}^{\lambda_a(p_z)}(\mathbf{r})}\Psi(\mathbf{r}),$$
$$\int \mathrm{d}\mathbf{r}\,|\Psi(\mathbf{r})|^2 = \int \mathrm{d}p_z\left[\sum_{l\in\mathbb{Z}}\int_0^\infty \left|\Phi_{l,p_z}\left(E^\perp\right)\right|^2 \mathrm{d}E^\perp + \sum_a \left|\Phi_{l_a,p_z}\right|^2\right].$$

10.2.2.2 Self-adjoint Schrödinger Operators with MSF

There is a family of s.a. three-dimensional Schrödinger operators $\hat{H}_{\lambda_*(p_z)}$ parameterized by real-valued functions $\lambda_*(p_z) \in \mathbb{S}(-\pi/2, \pi/2)$, $p_z \in (\mathbb{R})$, where λ_* are defined by (10.30).

The spectrum of $\hat{H}_{\lambda_*(p_z)}$ is given by

$$\operatorname{spec} \hat{H}_{\lambda_*(p_z)} = \left\{ p_z^2/2m_e + E_n^{\perp\lambda_*(p_z)},\ n \in \mathbb{Z}_+ \right\} \cup [\gamma M^{-1}, \infty),$$

where $E_n^{\perp\lambda_*(p_z)}$ are defined by (10.31) and (10.32) with the substitution $\lambda_* \to \lambda_*(p_z)$.

A complete system of generalized orthonormalized eigenfunctions of $\hat{H}_{\lambda_*(p_z)}$ consists of functions $\Psi_{p_z,l,n}(\mathbf{r})$, $l \neq l_*$, and $\Psi^{\lambda_*(p_z)}_{p_z,l_*,n}(\mathbf{r})$, $n \in \mathbb{Z}_+$,

$$\Psi_{p_z,l,n}(\mathbf{r}) = \frac{1}{2\pi\sqrt{\hbar\rho}} \mathrm{e}^{ip_z z/\hbar + \epsilon(\phi_0 - l)\varphi} U^{(1)}_{l,m(n,l)}(\rho),\ l \neq l_*, \tag{10.34}$$

where l_* are defined by (10.30), $m(n,l)$ is given by (10.29), and $U^{(1)}_{l,m}(\rho)$ are given by (10.20),

$$\Psi^{\lambda(p_z)}_{p_z,l_0,n}(\mathbf{r}) = \frac{1}{2\pi\sqrt{\hbar\rho}} \mathrm{e}^{ip_z z/\hbar + i\epsilon\phi_0\varphi} U^{(3)}_{\lambda(p_z),n}(\rho),\ \ \mu = 0,$$

$$\Psi^{\lambda_a(p_z)}_{p_z,l_a,n}(\rho) = \frac{1}{2\pi\sqrt{\hbar\rho}} \mathrm{e}^{ip_z z/\hbar + i\epsilon(\phi_0 - l_a)\varphi} U^{(2)}_{\lambda_a(p_z),n}(\rho),\ \mu > 0,$$

where $U^{(3)}_{\lambda(p_z),n}(\rho)$ and $U^{(2)}_{\lambda_a(p_z),n}(\rho)$ are given respective by (10.28) and (10.24) with the substitution $\lambda_* \to \lambda_*(p_z)$, so that

$$\check{H}\Psi_{p_z,l,n}(\mathbf{r}) = \left(p_z^2/2m_e + E^{\perp}_{n,l}\right)\Psi_{p_z,l,n}(\mathbf{r}),\ l \neq l_*,$$

$$\check{H}\Psi^{\lambda_*(p_z)}_{p_z,l_*,n}(\mathbf{r}) = \left(p_z^2/2m_e + E_n^{\perp\lambda_*(p_z)}\right)\Psi^{\lambda_*(p_z)}_{p_z,l_*,n}(\mathbf{r}), \tag{10.35}$$

where

$$E^{\perp}_{n,l} = \gamma M^{-1}[1 + 2n + 2\theta(l)\mu],\ l \leq n,\ l \neq l_*,\ n \in \mathbb{Z}_+. \tag{10.36}$$

We note that for $\lambda(p_z) = \lambda_a(p_z) = \pm\pi/2$, the energy eigenvalues and corresponding eigenfunctions $\Psi_{p_z,l,n}(\mathbf{r})$ are given by (10.34), (10.35), and (10.36) extended to all the values of l.

The corresponding inversion formulas have the form

$$\Psi(\mathbf{r}) = \int \mathrm{d}p_z \sum_{n\in\mathbb{Z}_+} \left[\sum_{l\in\mathbb{Z},\ l\neq l_*} \Phi_{p_z,l,n}\Psi_{p_z l,m(n,l)}(\mathbf{r}) + \sum_{l=l_*} \Phi_{p_z,l_*,n}\Psi^{\lambda_*(p_z)}_{p_z,l_*,n}(\mathbf{r}) \right],$$

$$\Phi_{p_z,l,n} = \int \mathrm{d}\mathbf{r}\overline{\Psi_{p_z,l,n}(\mathbf{r})}\Psi(\mathbf{r}), l \neq l_*, \Phi_{p_z,l_*,n} = \int \mathrm{d}\mathbf{r}\overline{\Psi^{\lambda(p_z)}_{p_z,l_*,n}(\mathbf{r})}\Psi(\mathbf{r}),$$

$$\int \mathrm{d}\mathbf{r}\, |\Psi(\mathbf{r})|^2 = \int \mathrm{d}p_z \sum_{l\in\mathbb{Z}} \sum_{n\in\mathbb{Z}_+} \left|\Phi_{p_z,l,n}\right|^2, \forall\Psi \in L^2\left(\mathbb{R}^3\right).$$

10.3 Self-adjoint Dirac Operators

10.3.1 Reduction to Radial Problem

Written in the form of the Schrödinger equation, the *Dirac equation with the MSF* reads[5]

$$i\frac{\partial\Psi(x)}{\partial t}=\check{H}\Psi(x),\ x=\left(x^0,\mathbf{r}\right),\ \mathbf{r}=\left(x^k,\ k=1,2,3\right),\ x^0=t,$$

where $\Psi(x)=\{\psi_\alpha(x),\ \alpha=1,\ldots,4\}$ is a bispinor (Dirac spinor) and $\check{H}$ is the *s.a. Dirac differential operation*,

$$\check{H}=\alpha\left(\check{\mathbf{p}}-q\mathbf{A}\right)+m_e\beta,$$

where $\check{\mathbf{p}}=-i\nabla,\nabla=\left(\partial_x,\partial_y,\partial_z\right)$, the vector potential $\mathbf{A}(x)$ is given by (10.2), $\alpha=\left(\gamma^0\gamma^k,k=1,2,3\right),\beta=\gamma^0$, and $\gamma^\mu,\mu=0,1,2,3$, are γ-matrices, chosen in the following representation:

$$\begin{aligned}&\gamma^0=\operatorname{diag}\left(\sigma^3,-\sigma^3\right),\ \gamma^1=\operatorname{diag}\left(i\sigma^2,-i\sigma^2\right),\ \gamma^2=\operatorname{diag}\left(-i\sigma^1,i\sigma^1\right),\\&\gamma^3=\operatorname{antidiag}\left(-I,I\right),\ \gamma^5=-i\gamma^0\gamma^1\gamma^2\gamma^3=-\operatorname{antidiag}\left(I,I\right),\end{aligned}$$

where $I=\operatorname{diag}(1,1)$ is the 2×2 identity matrix; for the definition of Pauli matrices, see Sect. 9.2.

The space of quantum states for the Dirac particle is the Hilbert space $\mathfrak{H}=\boldsymbol{L}^2\left(\mathbb{R}^3\right)$ of square-integrable bispinors $\Psi(\mathbf{r})$ with the scalar product

$$(\Psi_1,\Psi_2)=\int\mathrm{d}\mathbf{r}\Psi_1^+(\mathbf{r})\Psi_2(\mathbf{r}),\ \mathrm{d}\mathbf{r}=\mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3=\rho\,\mathrm{d}\rho\,\mathrm{d}\varphi\,\mathrm{d}z,$$

where ρ, φ, and z are cylindrical coordinates. The Hilbert space $\mathfrak{H}$ can be presented as

$$\mathfrak{H}=\sum_{\alpha=1}^{4}{}^{\oplus}\mathfrak{H}_\alpha,\ \ \mathfrak{H}_\alpha=L^2\left(\mathbb{R}^3\right).$$

Our first aim is to construct all s.a. Dirac operators (Dirac Hamiltonians) associated with the s.a. differential operation $\check{H}$ using the general approach presented in Chaps. 3 and 4. In addition, the construction is also based on the known spatial

[5]In this section, we set $c=\hbar=1$.

symmetry in the problem,[6] which allows for the separation of the cylindrical coordinates ρ, φ, and z.

Written in the cylindric coordinates, the differential operation $\check{H}$ then becomes

$$\check{H} = \operatorname{diag}\left(Y + m_e\sigma^3, Y - m_e\sigma^3\right) + \check{p}_z \operatorname{antidiag}\left(\sigma^3, \sigma^3\right),$$

where

$$Y = Q\left[\sigma^3\partial_\rho + \rho^{-1}\left(i\partial_\varphi + \epsilon_q\tilde{\phi}\right)\right],\ Q = \sigma^1\sin\varphi - \sigma^2\cos\varphi,\ Q^2 = 1,$$

and

$$\epsilon_q\tilde{\phi} = \epsilon(\phi_0 + \mu + \gamma\rho^2/2),\ \phi_0 = [\epsilon_B\phi] = \epsilon_B\phi - \mu,\ 0 \le \mu < 1,\ \gamma = e|B| > 0.$$

This operation commutes with the s.a. differential operations

$$\check{p}_z = -i\partial_z\ ,\ \check{S}_z = \gamma^5\left(\gamma^3 - m_e^{-1}\check{p}_z\right),$$
$$\check{J}_z = -i\partial_\varphi + \frac{1}{2}\Sigma^3 = \operatorname{diag}\left(\check{j}_z, \check{j}_z\right),\ \check{j}_z = -i\partial_\varphi + \sigma^3/2,$$

where $\Sigma^3 = \operatorname{diag}\left(\sigma^3, \sigma^3\right)$.

Now we pass to the p_z-representation for bispinors, $\Psi(\mathbf{r}) \to \tilde{\Psi}(p_z, \rho)$,

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{2\pi}}\int e^{ip_z z}\tilde{\Psi}(p_z, \rho)dp_z,\ \tilde{\Psi}(p_z, \rho) = \frac{1}{\sqrt{2\pi}}\int e^{-ip_z z}\Psi(\mathbf{x})dz.$$

In this representation, the operation $\check{J}_z$ is the same, while the operation $\check{H}$ and operation $\check{S}_z$ respectively become

$$\check{H} \to \check{H}(p_z) = \check{H} = \operatorname{diag}\left(Y + m_e\sigma^3, Y - m_e\sigma^3\right) + p_z \operatorname{antidiag}\left(\sigma^3, \sigma^3\right),$$
$$\check{S}_z \to \check{S}_z(p_z) = m_e^{-1}p_z \operatorname{antidiag}(I, I) + \operatorname{diag}(I, -I).$$

We decompose bispinor $\tilde{\Psi}(p_z, \rho)$ for a fixed p_z into two orthogonal components that are eigenvectors of the spin matrix $\hat{S}_z(p_z)$:

$$\tilde{\Psi}(p_z, \rho) = \tilde{\Psi}_1(p_z, \rho) + \tilde{\Psi}_{-1}(p_z, \rho),$$

[6] By *spatial symmetry*, we mean invariance under rotations around the solenoid axis and under translations along this axis.

where

$$\tilde{\Psi}_1(p_z,\rho) = \left(\frac{M+m_e}{2M}\right)^{1/2} \begin{pmatrix} \chi_1 \\ p_z (M+m_e)^{-1} \chi_1 \end{pmatrix} = \chi_1(p_z,\rho) \otimes e_1(p_z),$$
$$\tilde{\Psi}_{-1}(p_z,\rho) = \left(\frac{M+m_e}{2M}\right)^{1/2} \begin{pmatrix} -p_z (M+m_e)^{-1} \chi_{-1} \\ \chi_{-1} \end{pmatrix} = \chi_{-1}(p_z,\rho) \otimes e_{-1}(p_z),$$
$$e_1(p_z) = \left(\frac{M+m_e}{2M}\right)^{1/2} \begin{pmatrix} 1 \\ p_z (M+m_e)^{-1} \end{pmatrix},\ e_{-1}(p_z) = -i\sigma^2 e_1(p_z), \tag{10.37}$$

and $e_s(p_z)$, $s=\pm 1$, are two orthonormalized bispinors, $e_r^+(p_z)e_s^+(p_z) = \delta_{rs}$, and $\chi_s(p_z,\rho)$ are some doublets.

The space of bispinors $\tilde{\Psi}(p_z,\rho)$ with a fixed p_z is the direct orthogonal sum of two eigenspaces of $\hat{S}_z(p_z)$,

$$\hat{S}_z(p_z)\,\tilde{\Psi}_s(p_z,\rho) = s\frac{M}{m_e}\tilde{\Psi}_s(p_z,\rho),\ M = \sqrt{m_e^2+p_z^2},\ s=\pm 1.$$

We thus obtain a one-to-one correspondence $\Psi(\mathbf{r}) \iff \tilde{\Psi}_s(p_z,\rho) \iff \chi_s(p_z,\rho)$ between bispinors $\Psi(\mathbf{r})$ and pairs of doublets $\chi_s(p_z,\rho)$ such that

$$\|\Psi\|^2 = \sum_s \|\chi_s\|^2 = \sum_s \int \mathrm{d}p_z \mathrm{d}\rho\, \chi_s^+(p_z,\rho)\chi_s(p_z,\rho).$$

The differential operations $\check{H}$ and $\check{J}_z$ induce the differential operations $\check{\mathbf{h}}$ and $\check{j}_z$ in the space of doublets $\chi_s(p_z,\rho)$ as follows:

$$\check{H}\,(p_z)\,\tilde{\Psi}_s = \check{\mathbf{h}}\,(s,p_z)\,\chi_s \otimes e_s,\ \ \check{J}_z\,(p_z)\,\tilde{\Psi}_s = \check{j}_z\chi_s \otimes e_s,$$
$$\check{\mathbf{h}}\,(s,p_z) = Q\left[\sigma^3\partial_\rho + \rho^{-1}\left(i\partial_\varphi + \epsilon_q\tilde{\Phi}\right)\right] + sM\sigma^3.$$

The s.a. operator $\hat{j}_z$ associated with $\check{j}_z$ has a discrete spectrum, and its eigenvalues j_z are all half-integers labeled here by integers l as $j_z = \epsilon(\phi_0 - l + 1/2)$,

$$\hat{j}_z\xi_l(\varphi) = [\epsilon(\phi_0 - l + 1/2)]\xi_l(\varphi),\ l \in \mathbb{Z}.$$

It is convenient to represent vectors $\xi_l(\varphi) \equiv \xi_l(p_z,\rho,\varphi)$ of the corresponding eigenspaces, as

$$\xi_l(\varphi) = (2\pi)^{-1/2}\mathrm{e}^{i[\epsilon(\phi_0-l+1/2)-\sigma^3/2]\varphi}\vartheta_l = S_l(\varphi)\frac{1}{\sqrt{2\pi\rho}}F(l,p_z,\rho),$$
$$S_l(\varphi) = \mathrm{e}^{i\epsilon(\phi_0-l+1/2)\varphi}\mathrm{antidiag}\left(i\mathrm{e}^{i\varphi/2}, -\mathrm{e}^{-i\varphi/2}\right),\ S_l^+(\varphi)\,S_l(\varphi) = I, \tag{10.38}$$

where $\vartheta_l = \vartheta_l(p_z,\rho)$ and $F(l,p_z,\rho)$ are arbitrary doublets independent of φ.

The space of each of the doublets $\chi_s(p_z, \rho)$ is a direct orthogonal sum of the eigenspaces of the operator $\hat{j}_z$, which means that the doublets allow the representations

$$\chi_s(p_z, \rho) = \sum_{l \in \mathbb{Z}} \frac{1}{\sqrt{2\pi\rho}} S_l(\varphi) F(s, l, p_z, \rho),$$

where the factor $1/\sqrt{2\pi\rho}$ is introduced for later convenience.

Taking into account the relationships

$$\check{\mathbf{h}}(s, p_z) \frac{1}{\sqrt{\rho}} S_l = \frac{1}{\sqrt{\rho}} \left\{ Q\sigma^3 S_l \partial_\rho + \epsilon Q S_l \left[\rho^{-1}\varkappa_l + \gamma\rho/2\right] + sM\sigma^3 S_l \right\},$$
$$\check{\mathbf{h}}(s, p_z)\, \chi_s = \sum_{l \in \mathbb{Z}} \frac{1}{\sqrt{2\pi\rho}} S_l(\varphi) \check{h}(s, l)\, F(s, l, p_z; \rho),$$

where

$$\check{h}(s, l) = i\sigma^2 \partial_\rho + \epsilon(\gamma\rho/2 + \rho^{-1}\varkappa_l)\sigma^1 - sM\sigma^3,$$
$$\varkappa_l = l + \mu - 1/2, \tag{10.39}$$

we see that the operation $\check{\mathbf{h}}(s, p_z)$ induces an s.a. radial differential operation $\check{h}(s, l)$ (depending on the parameter p_z as well) in the space of doublets F.

In the Hilbert space[7] $\mathbb{L}^2(\mathbb{R}_+) = L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$ of doublets $F(\rho)$ (with p_z fixed), we define the initial symmetric radial Hamiltonian $\hat{h}(s, l)$ associated with the operation (10.39) and acting on the domain $D_{h(s,l)}$,

$$D_{h(s,l)} = \mathfrak{D}(\mathbb{R}_+) = \mathcal{D}(\mathbb{R}_+) \oplus \mathcal{D}(\mathbb{R}_+). \tag{10.40}$$

10.3.2 Solutions of Radial Equations

We first consider the radial equation

$$\left[\check{h}(s, l) - W\right] F(\rho) = 0 \tag{10.41}$$

and some of its useful solutions.

[7] See Sect. 9.2.

We let f and g denote the respective upper and lower components of doublets F, $F = (f \diagup g)$. Then (10.41) is equivalent to a set of *radial equations* for f and g,

$$
\begin{aligned}
&f' - \epsilon(\gamma\rho/2 + \rho^{-1}\varkappa_l)f + (W - sM)g = 0, \\
&g' + \epsilon(\gamma\rho/2 + \rho^{-1}\varkappa_l)g - (W + sM)f = 0,
\end{aligned} \tag{10.42}
$$

where the prime denotes the derivative with respect to ρ.

We let $\check{h}_+ = \check{h}_+(s,l)$ and $\check{h}_- = \check{h}_-(s,l)$ denote the differential operation $\check{h}$ with $\epsilon = 1$ and $\epsilon = -1$ respectively. We then have

$$
\begin{aligned}
\check{h}_+(s,l) &= i\sigma^2\partial_\rho + \left(\gamma\rho/2 + \rho^{-1}\varkappa_l\right)\sigma^1 - sM\sigma^3, \\
\check{h}_-(s,l) &= i\sigma^2\partial_\rho - \left(\gamma\rho/2 + \rho^{-1}\varkappa_l\right)\sigma^1 - sM\sigma^3 \\
&= i\sigma^2\left[i\sigma^2\partial_\rho + (\gamma\rho/2 + \rho^{-1}\varkappa)\sigma^1 + sM\sigma^3\right]\left(i\sigma^2\right)^+ \\
&= i\sigma^2\check{h}_+(-s,l)\left(i\sigma^2\right)^+.
\end{aligned}
$$

It follows that solutions $F_- = F_-(s,l,E_-(s);\rho)$ of $\left[\check{h}_- - E_-(s)\right]F_- = 0$ are bijectively related to solutions $F_+ = F_+(s,l,E_+(s);\rho)$ of the equation $\left[\check{h}_+ - E_+(s)\right]F_+ = 0$ as follows:

$$
F_-(s,l,E_-(s);\rho) = i\sigma^2 F_+(-s,l,E_+(-s);\rho),\ E_-(s) = E_+(-s).
$$

That is why we consider below the case $\epsilon = \operatorname{sgn}(qB) = 1$ only and omit the subscript "+".

The set (10.42) can be reduced to second-order differential equations for both f and g. For example, we have the following set of equations equivalent to (10.42):

$$
\begin{aligned}
&f'' - \left[(\gamma\rho/2)^2 + \frac{\varkappa_l(\varkappa_l - 1)}{\rho^2} - w + \gamma\left(\varkappa_l + \frac{1}{2}\right)\right]f = 0, \\
&g = (W - sM)^{-1}\left[-f' + (\gamma\rho/2 + \rho^{-1}\varkappa_l)f\right],\ w = W^2 - M^2.
\end{aligned} \tag{10.43}
$$

By the substitution

$$
f(\rho) = z^{a/2}\mathrm{e}^{-z/2}p(z),\ z = \gamma\rho^2/2,\ a = 1/2 \pm (\varkappa_l - 1/2),
$$

we reduce the first equation (10.43) to the equation for $p(z)$ that is the equation for confluent hypergeometric functions,

$$
\begin{aligned}
&z\partial_z^2 p + (\beta - z)\partial_z p - \alpha p = 0, \\
&\beta = a + 1/2, \\
&\alpha = a/2 + \varkappa_l/2 + 1/2 - w/2\gamma.
\end{aligned} \tag{10.44}
$$

Known solutions of (10.44) allow us to obtain solutions of (10.41).

In what follows, we use the following solutions $F_1(\rho; s, W)$, $F_2(\rho; s, W)$, and $F_3(\rho; s, W)$ of equation (10.41):

$$F_1 = \rho^{1/2-l-\mu} e^{-z/2} \begin{pmatrix} -(2\beta_1)^{-1}(W - sM)\rho\Phi(\alpha_1 + 1, \beta_1 + 1; z) \\ \Phi(\alpha_1, \beta_1; z) \end{pmatrix},$$

$$F_2 = \rho^{l+\mu-1/2} e^{-z/2} \begin{pmatrix} \Phi(\alpha_2, \beta_2; z) \\ (2\beta_2)^{-1}(W + sM)\rho\Phi(\alpha_2, \beta_2 + 1; z) \end{pmatrix},$$

$$F_3 = \rho^{1/2-l-\mu} e^{-z/2} \begin{pmatrix} 2^{-1}(W - sM)\rho\Psi(\alpha_1 + 1, \beta_1 + 1; z) \\ \Psi(\alpha_1, \beta_1; z) \end{pmatrix}, \tag{10.45}$$

where

$$\beta_1 = 1 - l - \mu,\ \alpha_1 = -w/2\gamma,\ \beta_2 = l + \mu,\ \alpha_2 = l + \mu - w/2\gamma,$$

$$\omega_1 = \omega_1(s, W) = \frac{2(\gamma/2)^{\beta_2}\Gamma(\beta_1)}{(W + sM)\Gamma(\alpha_1)},\ \omega_2 = \omega_2(W) = \frac{\Gamma(\beta_2)}{\Gamma(\alpha_2)}.$$

All the solutions F_1, F_2, and F_3 are real entire in W, and $F_3 = \omega_2 F_1 - \omega_1 F_2$.

The solutions (10.45) have the following asymptotic behavior at the origin and at infinity: As $\rho \to 0$, we have

$$F_1 = \rho^{1/2-l-\mu}\left(-(2\beta_1)^{-1}(W - sM)\rho/1\right)\tilde{O}\left(\rho^2\right),$$

$$F_2 = \rho^{l+\mu-1/2}\left(1/(2\beta_2)^{-1}(W + sM)\rho 1\right)\tilde{O}\left(\rho^2\right),$$

$$f_3 = \frac{(W - sM)\Gamma(\beta_1)}{2(\gamma/2)^{\beta_1}\Gamma(\alpha_1 + 1)}\rho^{l+\mu-1/2}\begin{cases} \tilde{O}\left(\rho^2\right),\ l \le -1, \\ \tilde{O}\left(\rho^{2-2\mu}\right),\ l = 0,\ \mu > 0, \\ \tilde{O}\left(\rho^2 \ln\rho\right),\ l = 0,\ \mu = 0, \end{cases}$$

$$g_3 = \frac{\Gamma(\beta_2)}{\Gamma(\alpha_2)}\rho^{1/2-l-\mu}\begin{cases} \tilde{O}\left(\rho^2\right),\ l \ge 1, \\ \tilde{O}\left(\rho^{2\mu}\right),\ l = 0,\ \mu > 0, \end{cases} \tag{10.46}$$

where $F_3 = (f_3/g_3)$.

As $\rho \to \infty$, we have

$$F_1 = \frac{(\gamma/2)^{\alpha_1-\beta_1}\Gamma(\beta_1)}{\Gamma(\alpha_1)}\rho^{-\varkappa_l+2\alpha_1-2\beta_1}e^{z/2}\left(\gamma\rho(W + sM)^{-1}/1\right)\tilde{O}\left(\rho^{-2}\right),$$

$$F_2 = \frac{(\gamma/2)^{\alpha_1}\Gamma(\beta_2)}{\Gamma(\alpha_2)}\rho^{\varkappa_l+2\alpha_1}e^{z/2}\left(1/(\gamma\rho)^{-1}(W + sM)\right)\tilde{O}\left(\rho^{-2}\right),$$

$$F_3 = (\gamma/2)^{-\alpha_1}\rho^{\varkappa_l-2\alpha_1}e^{-z/2}\left((\gamma\rho)^{-1}(W - sM)/1\right)\tilde{O}\left(\rho^{-2}\right).$$

We define the Wronskian $\mathrm{Wr}\left(F, \tilde{F}\right)$ of two doublets $F = (f \diagup g)$ and $\tilde{F} = \left(\tilde{f} \diagup \tilde{g}\right)$ by

$$\mathrm{Wr}\left(F, \tilde{F}\right) = f\tilde{g} - g\tilde{f} = iF\sigma^2\tilde{F}.$$

If $\left(\check{h} - W\right)F = \left(\check{h} - W\right)\tilde{F} = 0$, then $\mathrm{Wr}(F, \tilde{F}) = C =$ const. Solutions F and $\tilde{F}$ are linearly independent iff $C \neq 0$. It is easy to see that $\mathrm{Wr}(F_1, F_2) = -1$.

If $\mathrm{Im}\, W > 0$, solutions F_1, F_2, and F_3 are pairwise linearly independent,

$$\mathrm{Wr}(F_1, F_3) = \omega_1(W),\ \mathrm{Wr}(F_2, F_3) = \omega_2(W).$$

Taking the asymptotics of the linearly independent solutions F_1 and F_3 into account, we see that there are no square-integrable solutions of (10.41) with $\mathrm{Im}\, W \neq 0$ and $|l| \geq 1$ or $l = 0$, $\mu = 0$. This implies that in these cases, the deficiency indices of $\hat{h}\,(s, l)$ are zero. In the case $l = 0$, $\mu > 0$, the solution F_3 is square-integrable, which implies that the deficiency indices of $\hat{h}\,(s, 0)$ are $m_\pm = 1$.

For any l and μ, the asymptotic behavior of any solution F of (10.41) at the origin, as $\rho \to 0$, is no stronger than $\rho^{-|\varkappa_l|}$, that is, $F(\rho) = O\left(\rho^{-|\varkappa_l|}\right)$.

We now consider the inhomogeneous equation

$$\left[\check{h}\,(s, l) - W\right] F(\rho) = \Psi(\rho),\ \forall\Psi \in \mathbb{L}^2\left(\mathbb{R}_+\right),$$

see (5.34) from Chap. 5. Its general solution allows the representations

$$\begin{aligned} F(\rho) &= c_1 F_d(\rho; W) + c_2 F_3(\rho; W) + \omega_d^{-1} \\ &\quad\times\left[F_d(\rho; W)\int_\rho^\infty F_3(r; W)\Psi(r)\mathrm{d}r + F_3(\rho; W)\int_0^\rho F_d(r; W)\Psi(r)\mathrm{d}r\right], \\ \omega_d &= \mathrm{Wr}(F_d, F_3),\ \ d = \begin{cases} d = 1,\ l \leq 0, \\ d = 2,\ l \geq 1. \end{cases} \end{aligned} \tag{10.47}$$

A simple estimate of the integral terms on the right-hand side of (10.47) using the Cauchy–Schwarz inequality shows that they are bounded as $\rho \to \infty$. It follows that $F \in \mathbb{L}^2(\mathbb{R}_+)$ implies $c_1 = 0$.

For $|\varkappa_l| \geq 1/2$, an evaluation shows that as $\rho \to 0$, the integral terms are of order $O\left(\rho^{1/2}\right)$ (up to the factor $\ln\rho$ for $|\varkappa_l| = 1/2$). In this case, $F \in \mathbb{L}^2(\mathbb{R}_+)$ implies $c_2 = 0$, and we obtain

$$F(\rho) = \omega_d^{-1}\left[F_d(\rho; W)\int_\rho^\infty F_3(r; W)\Psi(r)\mathrm{d}r + F_3(\rho; W)\int_0^\rho F_d(r; W)\Psi(r)\mathrm{d}r\right]. \tag{10.48}$$

For $|\varkappa_l| \leq 1/2$, the doublet $F_3(\rho; W)$ is square-integrable, and a solution $F(\rho) \in \mathbb{L}^2(\mathbb{R}_+)$ allows the representation

$$F(\rho) = b\omega_1^{-1} F_1(\rho; W) + c_2 F_3(\rho; W) + \omega_1^{-1} \\ \times \left[F_3(\rho; W) \int_0^\rho F_1(r; W)\Psi(r)\mathrm{d}r - F_1(\rho; W) \int_0^\rho F_3(r; W)\Psi(r)\mathrm{d}r \right], \tag{10.49}$$

so that as $\rho \to 0$, we have

$$F(\rho) = \omega_1^{-1} \left(\int_0^\infty F_3(r; W)\Psi(r)\mathrm{d}r \right) F_1(\rho; W) + c_2 F_3(\rho; W) + O\left(\rho^{1/2}\right).$$

Following Sect. 5.3, we will use representations (10.47)–10.49) to obtain Green's functions for s.a. radial Hamiltonians.

10.3.3 Self-adjoint Radial Hamiltonians

We proceed to the construction of s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(s,l)$ as s.a. extensions of the initial symmetric radial operators $\hat{h}(s,l)$ (10.40) and analyze the corresponding spectral problems.

The action of all of the following operators associated with the differential operations $\check{h}(s,l)$ is given by $\check{h}(s,l)$; therefore we cite only their domains.

We begin with the adjoint $\hat{h}^+(s,l)$ of $\hat{h}(s,l)$. Its domain D_{h^+} is the natural domain $D^*_{\check{h}(s,l)}(\mathbb{R}_+)$ for $\check{h}(s,l)$,

$$D^*_{\check{h}(s,l)}(\mathbb{R}_+) = \left\{ F_*(\rho) : F_* \text{ are a.c., } F_*, \check{h}(s,l)\, F_* \in \mathbb{L}^2(\mathbb{R}_+) \right\}.$$

The quadratic asymmetry form $\varDelta_{h^+}(F_*)$ of $\hat{h}^+(s,l)$ is expressed in terms of the local quadratic form

$$[F_*, F_*](\rho) = \overline{g(\rho)} f(\rho) - \overline{f(\rho)} g(\rho), \;\; F_* = (f \diagup g),$$

as follows:

$$\varDelta_{h^+}(F_*) = \left(F_*, \hat{h}^+ F_* \right) - \left(\hat{h}^+ F_*, F_* \right) = -\left[F_*, F_* \right](\rho)\big|_0^\infty .$$

One can prove that $\lim_{\rho\to\infty} F_*(\rho) = 0$ for any $F_* \in D^*_{\check{h}}(\mathbb{R}_+)$. Indeed, because F_* and $\check{h}(s,l)\, F_*$ are square-integrable at infinity, the combination

$$F_*' - (\gamma\rho/2)\,\sigma^3 F_* = -i\sigma^2\left[\check{h}(s,l)\, F_* - (\varkappa_l/\rho)\sigma^1 F_* + sM\sigma^3 F_*\right]$$

is also square-integrable at infinity. This implies that f and $f' - (\gamma\rho/2)\, f$, together with g and $g' + (\gamma\rho/2)\, g$, are square-integrable at infinity. Let us consider the identity

$$|f(\rho)|^2 = \int_a^\rho \left[\overline{\partial f(r)}\, f(r) + \overline{f(r)}\partial f(r)\right] \mathrm{d}r + \gamma\int_a^\rho r|f(r)|^2 \mathrm{d}r + |f(a)|^2,$$

where $\partial = \partial_\rho - \gamma\rho/2$. The right-hand side of this identity has a limit (finite or infinite) as $\rho \to \infty$. Therefore, $|f(\rho)|$ also has a limit as $\rho \to \infty$. This limit has to be zero because $f(\rho)$ is square-integrable at infinity. In the same manner, one can verify that $g(\rho) \to 0$ as $\rho \to \infty$.

To analyze the behavior of F_* at the origin, we consider the relationship

$$\Psi = \check{h}(s,l)\, F_*, \Psi, F_* \in \mathbb{L}^2(\mathbb{R}_+),$$

or

$$f' - \left(\gamma\rho/2 + \rho^{-1}\varkappa_l\right) f = -\chi_2,\ g' + \left(\gamma\rho/2 + \rho^{-1}\varkappa_l\right) g = \chi_1,$$
$$\chi = (\chi_1 \diagup \chi_2) = \Psi + sM\sigma^3 F_* \in \mathbb{L}^2(\mathbb{R}_+),$$

as an equation for F_* at a given χ. The general solution of these equations allows the representation

$$f(\rho) = \rho^{\varkappa_l}\mathrm{e}^{\gamma\rho^2/4}\left[c_1 + \int_\rho^\infty r^{-\varkappa_l} e^{-\gamma r^2/4}\chi_2(r)\mathrm{d}r\right],$$
$$g(\rho) = \rho^{-\varkappa_l}\mathrm{e}^{-\gamma\rho^2/4}\left[c_2 + \int_{\rho_0}^\rho r^{\varkappa_l} e^{\gamma r^2/4}\chi_1(r)\mathrm{d}r\right]. \tag{10.50}$$

It turns out that the asymptotic behavior of the functions f and g at the origin crucially depends on the value of l. Therefore, our exposition is naturally divided into subsections related to the corresponding regions. We distinguish three regions of l.

10.3.3.1 First Region: $\varkappa_l \leq -1/2$

In this region, we have

$$l \leq \begin{cases} -1, & \mu > 0, \\ 0, & \mu = 0. \end{cases}$$

The representation (10.50) allows the estimation of the asymptotic behavior of doublets $F_* \in D^*_{\check{h}(s,l)}(\mathbb{R}_+)$ as $\rho \to 0$ for the first region. For $f(\rho)$, we have

$$f(\rho) = \rho^{-|\varkappa_l|} e^{\gamma\rho^2/4}\left[\tilde{c}_1 - \int_0^\rho r^{|\varkappa_l|} e^{-\gamma r^2/4}\chi_2(r)dr\right]$$
$$= \tilde{c}_1\rho^{-|\varkappa_l|} + O\left(\rho^{1/2}\right),\ \tilde{c}_1 = c_1 + \int_0^\infty r^{|\varkappa_l|} e^{-\gamma r^2/4}\chi_2(r)dr.$$

The condition $f \in L^2(\mathbb{R}_+)$ implies $\tilde{c}_1 = 0$, and therefore, $f(\rho) = O\left(\rho^{1/2}\right)$ as $\rho \to 0$. As to $g(\rho)$, we obtain as $\rho \to 0$,

$$g(\rho) = \begin{cases} O\left(\rho^{1/2}\right), \varkappa_l < -1/2, \\ O\left(\rho^{1/2}\ln\rho\right), \varkappa_l = -1/2 (l = 0, \mu = 0). \end{cases}$$

Thus, $F_*(\rho) \to 0$ as $\rho \to 0$, which implies that $\Delta_{h^+}(F_*) = 0$, $\forall F_* \in D^*_{\check{h}(s,l)}(\mathbb{R}_+)$. This means that the deficiency indices of each of the symmetric operators $\hat{h}(s,l)$ in the first region are zero. Therefore, there exists only one s.a. extension $\hat{h}_{(1)}(s,l) = \hat{h}^+(s,l)$ of $\hat{h}(s,l)$, that is, a unique s.a. radial Hamiltonian with given s and l; its domain is the natural domain, $D_{h_{(1)}(s,l)} = D^*_{\check{h}(s,l)}(\mathbb{R}_+)$.

The representation (10.48) with $d = 1$ implies that the Green's function (see (5.35)) of the s.a. Hamiltonian $\hat{h}_{(1)}(s,l)$ is given by

$$G\left(\rho,\rho';W\right) = \omega_1^{-1}(W)\begin{cases} F_3(\rho;W)\otimes F_1\left(\rho';W\right), \rho > \rho', \\ F_1(\rho;W)\otimes F_3\left(\rho';W\right), \rho < \rho'. \end{cases}$$

Unfortunately, we cannot use representation (10.45) for F_3 as a sum of two terms directly for all the values of μ because both are singular at $\mu = 0$ (although the sum is not). To cover the total range of μ, we use another representation for F_3.

We let $F_{il}(\rho;W)$ denote the functions $F_i(\rho;W)$, $i = 1,2,3$, with a fixed l and represent F_{3l} as

$$F_{3l} = \omega_1[A_{1l}F_{1l} + F_{4l}],\ A_{1l} = A_{1l}(W) = \Omega_1(W) - \Gamma(\beta_2)P_{1l}(W),$$
$$F_{4l} = F_{4l}(\rho;W) = \Gamma(\beta_2)P_{1l}(W)F_{1l}(\rho;W) - F_{2l}(\rho;W),$$
$$\Omega_1(W) = \frac{\omega_2(W)}{\omega_1(W)},\ P_{1l}(W) = \frac{(W+sM)(\gamma/2)^{|l|}\Gamma(\alpha_1)}{2|l|!\Gamma(\alpha_1 - |l|)}.$$

Using the relationship (8.27), we can verify that

$$\Gamma^{-1}(\beta_2)F_{2l}(\rho;W)\big|_{\mu\to 0} = P_{1l}(W)F_{1l}(\rho;W)|_{\mu=0}.$$

Taking the latter relationship into account, it is easy to see that in the first region, A_{1l} and F_{4l} are finite for $\mu \geq 0$, as well as ω_1 and F_{1l}, and also that $P_{1l}(E)$ and $F_{4l}(\rho; E)$ are real.

The Green's function is then represented as

$$G\left(\rho, \rho'; W\right) = A_{1l}(W) F_{1l}(\rho; W) \otimes F_{1l}\left(\rho'; W\right) + \begin{cases} F_{4l}(\rho; W) \otimes F_{1l}\left(\rho'; W\right), \rho > \rho', \\ F_{1l}(\rho; W) \otimes F_{4l}\left(\rho'; W\right), \rho < \rho', \end{cases} \tag{10.51}$$

for all $\mu \geq 0$.

We choose the guiding functional $\Phi(F; W)$ for the s.a. operator $\hat{h}_{(1)}(s, l)$ in the form (5.33) with $U = F_1$ and $\mathbb{D} = D_r(\mathbb{R}_+) \cap D_{h_{(1)}(s,l)}$. To prove that the guiding functional is simple, it suffices to verify only property (ii) (see Chap. 5). Let $\Phi(F_0; E_0) = 0$, where $F_0 \in \mathbb{D}$, and let

$$\tilde{F}(\rho) = F_1(\rho; E_0) \int_\rho^\infty F(r) F_0(r) \mathrm{d}r + F(\rho) \int_0^\rho F_1(r; E_0) F_0(r) \mathrm{d}r$$

be a solution of the equation $\left(\check{h}(s, l) - E_0\right) \tilde{F} = F_0$, where $F(\rho)$ is any solution of (10.41) with $W = E_0$ satisfying the condition $\mathrm{Wr}(F_1, F) = 1$. It is then easy to verify that $\tilde{F}(\rho) \in \mathbb{D}$. Therefore, the spectrum of $\hat{h}_{(1)}(s, l)$ is simple.

Using representation (10.51) for the Green's function, we obtain the derivative of the spectral function,

$$\sigma'(E) = \pi^{-1} \operatorname{Im} A_{1l}(E + i0). \tag{10.52}$$

It is easy to prove that $\operatorname{Im} A_{1l}(E + i0)$ is continuous in μ for $\mu \geq 0$, so that it is sufficient to obtain $\sigma'(E)$ only for the case $\mu > 0$, where (10.52) is simpler,

$$\sigma'(E) = \left. \frac{(W + sM)(\gamma/2)^{-\beta_2} \Gamma(\beta_2)}{2\pi \Gamma(\beta_1) \Gamma(\alpha_2)} \right|_{W=E} \operatorname{Im} \Gamma(\alpha_1)|_{W=E+i0}. \tag{10.53}$$

It is easy to see that $\sigma'(E)$ may differ from zero only at the points E_k defined by the relationship $\alpha_1 = -k$ ($\Gamma(\alpha_1) = \infty$), or $M^2 - E_k^2 = -2\gamma k$, which yields

$$E_k = \pm M_k, \ M_0 = M, \ k \in \mathbb{Z}_+, \ M_x = \sqrt{M^2 + 2\gamma x}. \tag{10.54}$$

The presence of the factor $(E + sM)$ on the right-hand side of (10.53) implies that the points $E = -sM = -sM_0$ do not belong to the spectrum of $\hat{h}_{(1)}(s, l)$.

In what follows it is convenient to change the numeration of the spectrum points. To this end, let us introduce an index $\mathfrak{n}(s)$:

$$\mathfrak{n}(s) \in \mathcal{Z}(s) = \left\{n_\zeta(s)\right\},\ \zeta = \pm\,,$$
$$n_+(s) \in \begin{cases} \mathbb{Z}_+, & s = 1, \\ \mathbb{N}, & s = -1, \end{cases} \quad n_-(s) \in \begin{cases} -\mathbb{N}, & s = 1, \\ \mathbb{Z}_-, & s = -1. \end{cases} \tag{10.55}$$

Then we can write

$$E_k = \pm M_k \Longrightarrow E_{\mathfrak{n}(s)} = \zeta M_{|\mathfrak{n}(s)|},\ \mathfrak{n}(s) \in \mathcal{Z}(s).$$

Finally, using the introduced notation, we obtain for $\sigma'(E)$,

$$\sigma'(E) = \sum_{\mathfrak{n}(s)\in\mathcal{Z}(s)} Q^2_{\mathfrak{n}(s)}\delta\left(E - E_{\mathfrak{n}(s)}\right),$$
$$Q_{\mathfrak{n}(s)} = \sqrt{\frac{(\gamma/2)^{\beta_1}\,\Gamma\left(\beta_1 + |\mathfrak{n}(s)|\right)\left(1 + sME_k^{-1}\right)}{|\mathfrak{n}(s)|!\Gamma^2(\beta_1)}},\ \beta_1 = 1 + |l| - \mu.$$

Thus, the simple spectrum of $\hat{h}_{(1)}(s,l)$ is given by spec $\hat{h}_{(1)}(s,l) = \left\{E_{\mathfrak{n}(s)},\ \mathfrak{n}(s) \in \mathcal{Z}(s)\right\}$. The eigenvectors

$$\overset{I}{U}_{\mathfrak{n}(s)} = \overset{I}{U}_{\mathfrak{n}(s)}(s,l,p_z;\rho) = Q_{\mathfrak{n}(s)}F_1(\rho;E_{\mathfrak{n}(s)}),\ \mathfrak{n}(s) \in \mathcal{Z}(s), \tag{10.56}$$

of $\hat{h}_{(1)}(s,l)$ form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$ of doublets $F(\rho)$; see (5.36).

10.3.3.2 Second Region: $\varkappa_l \geq 1/2$

In this region, we have $l \geq 1$.

Here the representation (10.50) yields the following estimates for the asymptotic behavior of doublets $F_* \in D^*_{\check{h}(s,l)}(\mathbb{R}_+)$ as $\rho \to 0$:

$$f(\rho) = \begin{cases} O\left(\rho^{1/2}\right), \varkappa_l > 1/2, \\ O\left(\rho^{1/2}\ln\rho\right), \varkappa_l = 1/2, \end{cases}$$
$$g(\rho) = O\left(\rho^{1/2}\right).$$

It follows that $F_*(\rho) \to 0$ as $\rho \to 0$, which implies that $\Delta_{h^+}(F_*) = 0, \forall F_* \in D^*_{\check{h}(s,l)}(\mathbb{R}_+)$. This means that the deficiency indices of each symmetric operator

$\hat{h}\,(s,l)$ are zero in the second region. Therefore, there exists only one s.a. extension $\hat{h}_{(2)}\,(s,l) = \hat{h}^{+}\,(s,l)$ of $\hat{h}\,(s,l)$, that is, a unique s.a. radial Hamiltonian with given s and l, whose domain is the natural domain, $D_{h_{(2)}(s,l)} = D^{*}_{\check{h}(s,l)}\,(\mathbb{R}_{+})$.

The representation (10.48) with $d = 2$ implies that the Green's function for the s.a. Hamiltonian $\hat{h}_{(2)}\,(s,l)$ is given by

$$G\left(\rho,\rho';W\right) = \omega_2^{-1}(W)\begin{cases} F_{3l}(\rho;W)\otimes F_{2l}\left(\rho';W\right), \rho>\rho', \\ F_{2l}(\rho;W)\otimes F_{3l}\left(\rho';W\right), \rho<\rho'. \end{cases}$$

Again, the representation (10.45) for F_3 as a sum of two terms is not applicable directly for $\mu = 0$. We therefore use the following representation for F_3:

$$\begin{aligned} F_{3l} &= \omega_2\left(F_{5l} - A_{2l}F_{2l}\right), A_{2l} = A_{2l}(W) = \varOmega_2(W) + \varGamma(\beta_1)P_{2l}(W), \\ F_{5l} &= F_{5l}(\rho;W) = F_{1l}(\rho;W) + \varGamma(\beta_1)P_{2l}(W)F_{2l}(\rho;W), \\ \varOmega_2(W) &= \frac{\omega_1(W)}{\omega_2(W)},\ P_{2l}(W) = \frac{(W-sM)(\gamma/2)^{l-1}\varGamma(\alpha_1+l)}{2(l-1)!\,\varGamma(\alpha_1+1)}. \end{aligned}$$

Using (10.54), one can verify that

$$\varGamma^{-1}(\beta_1)F_{1l}(\rho;W)\big|_{\mu\to 0} = -\,P_{2l}(W)F_{2l}(\rho;W)\big|_{\mu=0}.$$

Taking the latter relationship into account, it is easy to see that A_{2l} and F_{5l} are finite for $\mu \geq 0$, as well as ω_2 and F_{2l}, and $P_{2l}(E)$ and $F_{5l}(\rho;E)$ are real.

The Green's function is then represented as

$$\begin{aligned} G\left(\rho,\rho';W\right) = &-A_{2l}(W)F_{2l}(\rho;W)\otimes F_{2l}\left(\rho';W\right) \\ &+\begin{cases} F_{5l}(\rho;W)\otimes F_{2l}\left(\rho';W\right), \rho>\rho', \\ F_{2l}(\rho;W)\otimes F_{5l}\left(\rho';W\right), \rho<\rho', \end{cases} \end{aligned} \quad (10.57)$$

for all $\mu \geq 0$.

We choose the guiding functional $\varPhi(F;W)$ in the form (5.33) with $U = F_2$ and $\mathbb{D} = D_r(\mathbb{R}_{+}) \cap D_{h_{(2)}(s,l)}$. Its simplicity is proved in a similar way to the first region case and implies that the spectrum of $\hat{h}_{(2)}\,(s,l)$ is simple.

Using representation (10.57), we obtain that the derivative $\sigma'(E)$ of the spectral function is given by

$$\sigma'(E) = -\pi^{-1}\,\mathrm{Im}\,A_{2l}(E+i0). \quad (10.58)$$

It is easy to prove that $\mathrm{Im}\, A_{2l}(E + i0)$ is continuous in μ for $\mu \geq 0$, so that it is sufficient to obtain $\sigma'(E)$ only for the case $\mu > 0$, where the right-hand side of (10.58) is simpler,

$$\sigma'(E) = \left. \frac{(W - sM)\,(\gamma/2)^{\beta_2}\,\Gamma(\beta_1)}{\pi\gamma\Gamma(\beta_2)\Gamma(1+\alpha_1)} \right|_{W=E} \mathrm{Im}\,\Gamma\,(\alpha_2)|_{W=E+i0}.$$

It is easy to see that $\sigma'(E)$ may differ from zero only at the points E_k defined by the relationship $\alpha_2 = -k$ ($\Gamma\,(\alpha_2) = \infty$) or by the relationship

$$M^2 - E_k^2 + 2\gamma(l + \mu) = -2\gamma k\,,\ k \in \mathbb{Z}_+\,,$$

which yields $E_k = \pm M_{k+l+\mu},\ k \in \mathbb{Z}_+$, where M_x is defined by (10.54). All such points E_k are spectrum points.

It is convenient to change indexing k for $\mathfrak{n}(s)$, defined by (10.55),

$$E_k \Longrightarrow E_{\mathfrak{n}(s)} = \zeta M_{|\mathfrak{n}(s)|+\mu},$$
$$\left\{\mathfrak{n}(s) \in \mathcal{Z}(s),\ |\mathfrak{n}(s)| \geq l\right\}\ \left(n_\zeta(s) = \zeta(k+l),\ k \in \mathbb{Z}_+\right).$$

Thus, we finally obtain

$$\sigma'(E) = \sum_{\mathfrak{n}(s)\in\mathcal{Z},|\mathfrak{n}(s)|\geq l} Q^2_{\mathfrak{n}(s)}\delta\left(E - E_{\mathfrak{n}(s)}\right),$$
$$Q_{\mathfrak{n}(s)} = \sqrt{\frac{(\gamma/2)^{l+\mu}\,\Gamma(|\mathfrak{n}(s)|+\mu)\left(1 - sME^{-1}_{\mathfrak{n}(s)}\right)}{(|\mathfrak{n}(s)|-l)!\Gamma^2(l+\mu)}}\,.$$

The simple spectrum of $\hat{h}_{(2)}\,(s,l)$ is given by

$$\mathrm{spec}\,\hat{h}_{(2)}\,(s,l) = \left\{E_{\mathfrak{n}(s)},\ \mathfrak{n}(s) \in \mathcal{Z},\ |\mathfrak{n}(s)| \geq l\right\}.$$

The eigenvectors

$$\overset{II}{U}_{\mathfrak{n}(s)} = \overset{II}{U}_{\mathfrak{n}(s)}\,(s,l,p_z;\rho) = Q_{\mathfrak{n}(s)}F_2\left(\rho; E_{\mathfrak{n}(s)}\right), \quad \mathfrak{n}(s) \in \mathcal{Z}(s), \tag{10.59}$$

of $\hat{h}_{(2)}\,(s,l)$ form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$ of doublets $F\,(\rho)$.

10.3.3.3 Third Region: $|\varkappa_l| < 1/2$

In this region $l = l_0 = 0$, and $\varkappa_l$ is reduced to $\varkappa_0 = \mu - 1/2$, $\mu > 0$.

Representation (10.50) yields the following asymptotic behavior of doublets $F_* \in D^*_{\check{h}(s,l_0)}(\mathbb{R}_+)$ as $\rho \to 0$:

$$F_*(\rho) = \begin{cases} f(\rho) = c_1(m_e\rho)^{\varkappa_0} \\ g(\rho) = c_2(m_e\rho)^{-\varkappa_0} \end{cases} + O\left(\rho^{1/2}\right).$$

It follows that $\Delta_{h^+}(F_*) = \overline{c_2}c_1 - \overline{c_1}c_2$. Such a representation for the quadratic form $\Delta_{h^+}(F_*)$ implies that the deficiency indices of the initial symmetric operator $\hat{h}(s, l_0)$ are $m_\pm = 1$. The condition $\Delta_{h^+}(F_*) = 0$ yields asymptotic boundary conditions as $\rho \to 0$,

$$F(\rho) = C\begin{pmatrix} (m_e\rho)^{\varkappa_0}\cos\lambda \\ (m_e\rho)^{-\varkappa_0}\sin\lambda \end{pmatrix} + O\left(\rho^{1/2}\right), \tag{10.60}$$

with a fixed $\lambda \in \mathbb{S}(-\pi/2, \pi/2)$ (note that λ depends on s and p_z, $\lambda = \lambda(s, p_z)$) that define a maximum subspace in $D^*_{\check{h}(s,l_0)}(\mathbb{R}_+)$ where $\Delta_{h^+} = 0$. This subspace is just the domain of an s.a. extension of $\hat{h}(s, l_0)$ (see Chap. 4 and problems from Chaps. 6, 7, and 8).

We thus obtain that there exists a one-parameter $U(1)$ family of s.a. radial Hamiltonians $\hat{h}_\lambda(s, l_0)$ parameterized by the real parameter $\lambda \in \mathbb{S}(-\pi/2, \pi/2)$. These Hamiltonians are specified by the domains

$$D_{h_\lambda(s,l_0)} = \left\{F(\rho) : F(\rho) \in D^*_{\check{h}_\lambda(s,l_0)}(\mathbb{R}_+),\ F \text{ satisfy } (10.60)\right\}.$$

According to representation (10.49), which certainly holds for the doublets F belonging to $D_{h_\lambda(s,l_0)}$, and (10.46), the asymptotic behavior of F as $\rho \to 0$ reads

$$F = \begin{pmatrix} -c_2\omega_1\rho^{\varkappa_0} \\ \left(b\omega_1^{-1} + c_2\omega_2\right)\rho^{-\varkappa_0} \end{pmatrix} + O\left(\rho^{1/2}\right).$$

On the other hand, F satisfies boundary conditions (10.60), whence it follows that there must be

$$c_2 = -\frac{b\cos\lambda}{\omega_1\omega_{(\lambda)}},\quad \omega_{(\lambda)} = \omega_2\cos\lambda + m_e^{-2\varkappa_0}\omega_1\sin\lambda. \tag{10.61}$$

Then representation (10.49) for F with c_2 given by (10.61) implies that the Green's function of $\hat{h}_\lambda(s, l_0)$ is given by

$$\begin{aligned} G\left(\rho, \rho'; W\right) &= \Omega^{-1}(W)F_{(\lambda)}(\rho; W) \otimes F_{(\lambda)}\left(\rho'; W\right) \\ &\quad + \begin{cases} \tilde{F}_{(\lambda)}(\rho; W) \otimes F_{(\lambda)}\left(\rho'; W\right),\ \rho > \rho', \\ F_{(\lambda)}(\rho; W) \otimes \tilde{F}_{(\lambda)}\left(\rho'; W\right), \rho < \rho', \end{cases} \end{aligned} \tag{10.62}$$

where

$$F_{(\lambda)}(\rho; W) = m_e^{-\varkappa_0} F_1(\rho; W) \sin\lambda + m_e^{\varkappa_0} F_2(\rho; W) \cos\lambda,$$
$$\tilde{F}_{(\lambda)}(\rho; W) = m_e^{-\varkappa_0} F_1(\rho; W) \cos\lambda - m_e^{\varkappa_0} F_2(\rho; W) \sin\lambda,$$
$$\Omega(W) = \frac{\omega_{(\lambda)}(W)}{\tilde{\omega}_{(\lambda)}(W)},\ m_e^{\varkappa_0} F_3 = \tilde{\omega}_{(\lambda)} F_{(\lambda)} + \omega_{(\lambda)} \tilde{F}_{(\lambda)},$$
$$\tilde{\omega}_{(\lambda)}(W) = \omega_2 \sin\lambda - m_e^{-2\varkappa_0} \omega_1 \cos\lambda.$$

We note that the doublets $F_{(\lambda)}(\rho; W)$ and $\tilde{F}_{(\lambda)}(\rho; W)$ are real entire in W, and the doublet $F_{(\lambda)}(\rho; W)$ satisfies asymptotic s.a. boundary conditions (10.60).

Here, we choose the guiding functional $\Phi(F; W)$ in the form (5.33) with $U = F_{(\lambda)}$ and $\mathbb{D} = D_r(\mathbb{R}_+) \cap D_{h_\lambda(s,l_0)}$. Its simplicity is proved similarly to the first and second regions and implies that the spectrum of $\hat{h}_\lambda\,(s, l_0)$ is simple.

Using the representation (10.62) for the Green's function, we obtain that the derivative $\sigma'(E)$ of the spectral function is given by $\sigma'(E) = \pi^{-1}\operatorname{Im}\Omega^{-1}(E + i0)$. Because $\Omega(E)$ is real, $\sigma'(E)$ differs from zero only at the points E_k defined by the relation $\Omega(E_k) = 0$, and we obtain

$$\sigma'(E) = \sum_{k\in\mathbb{Z}} Q_k^2 \delta(E - E_k),\ \ Q_k = \left[-\Omega'(E_k)\right]^{-1/2},\ \Omega'(E_k) < 0.$$

Thus, the simple spectrum of $\hat{h}_\lambda\,(s, l_0)$ is given by spec $\hat{h}_\lambda\,(s, l_0) = \{E_k,\ k \in \mathbb{Z}\}$. The eigenvectors

$$\overset{III}{U_k} = \overset{III}{U_k}\,(\lambda, s, p_z; \rho) = Q_k F_{(\lambda)}(\rho; E_k),\ k \in \mathbb{Z}, \tag{10.63}$$

of $\hat{h}_\lambda\,(s, l_0)$ form a complete and orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$ of doublets $F\,(\rho)$.

Let us study the spectrum in greater detail.

I. First, we consider the case $\lambda = \pi/2$. In this case we have

$$F_{(\pi/2)}(\rho; W) = m_e^{-\varkappa_0} F_1(\rho; W),\ \ \Omega(W) = m_e^{-2\varkappa_0} \omega_1(W)\omega_2^{-1}(W),$$

and

$$\sigma'(E) = \left.\frac{m_e^{2\varkappa_0}\Gamma(\beta_2)(W + sM)}{2\pi\,(\gamma/2)^{\beta_2}\,\Gamma(\beta_1)\Gamma(\alpha_2)}\right|_{W=E} \operatorname{Im}\Gamma\,(\alpha_1)|_{W=E+i0}. \tag{10.64}$$

As in the first region, $\sigma'(E)$ differs from zero only at the points (for which we will use the notation $\mathcal{E}_k$) defined by the relationship $\alpha_1 = -k$ ($\Gamma(\alpha_1) = \infty$), or by

$$\frac{M^2 - \mathcal{E}_k^2}{2\gamma} = -k,\ E_k = \pm M_k,\ k \in \mathbb{Z}_+.$$

The presence of the factor $(E + sM)$ on the right-hand side of (10.64) implies that the points $E = -sM = -sM_0$ do not belong to the spectrum of $\hat{h}_{\pi/2}(s, l_0)$. Thus,

$$\mathcal{E}_k = (\operatorname{sgn} k) M_{|k|},\ |k| \geq 1,\ \ \mathcal{E}_0 = sM,\ k \in \mathbb{Z}.$$

Using (10.55), we change the indexing of the spectrum points,

$$\mathcal{E}_k \Longrightarrow \mathcal{E}_{\mathfrak{n}(s)} = \zeta M_{|\mathfrak{n}(s)|},\ \mathfrak{n} = \mathfrak{n}(s) \in \mathcal{Z}(s).$$

Then we finally obtain

$$\sigma'(E) = \sum_{\mathfrak{n}(s) \in \mathcal{Z}(s)} m_e^{2\varkappa_0} Q^2_{\pi/2|\mathfrak{n}(s)} \delta\left(E - \mathcal{E}_{\mathfrak{n}(s)}\right),$$

$$Q_{\pi/2|\mathfrak{n}(s)} = \sqrt{\frac{\Gamma(|\mathfrak{n}(s)| + 1 - \mu)\left(1 + sM\mathcal{E}^{-1}_{\mathfrak{n}(s)}\right)}{(\gamma/2)^{\beta_2}\,|\mathfrak{n}|!\,\Gamma^2(1-\mu)}}.$$

Thus, the simple spectrum of $\hat{h}_{\pi/2}(s, l_0)$ is given by spec $\hat{h}_{\pi/2}(s, l_0) = \left\{\mathcal{E}_{\mathfrak{n}(s)},\ \mathfrak{n}(s) \in \mathcal{Z}(s)\right\}$. The eigenvectors

$$\overset{III}{U}_{\pi/2|\mathfrak{n}(s)} = \overset{III}{U}_{\pi/2|\mathfrak{n}(s)}(\pi/2, s, l_0, p_z; \rho) = Q_{\pi/2|\mathfrak{n}(s)} F_1\left(\rho; \mathcal{E}_{\mathfrak{n}(s)}\right), \mathfrak{n}(s) \in \mathcal{Z}(s),$$

of $\hat{h}_{\pi/2}(s, l_0)$ form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$ of doublets $F(\rho)$.

We note that the spectrum, spectral function, and eigenfunctions of $\hat{h}_{\pi/2}(s, l_0)$ can be obtained from the respective expressions from the first region, $\varkappa_l \leq -1/2$, by the substitution $l = 0$. We also note that for $\mu < 1/2$, the function $F_{(\pi/2)}(\rho; W) = m_e^{-\varkappa_0} F_1(\rho; W)$ has a minimal singularity in the family of functions $F_{(\lambda)}(\rho; W)$; in fact, it is nonsingular. For $\mu > 1/2$, the function $F_{(0)}(\rho; W) = m_e^{\varkappa_0} F_2(\rho; W)$ has a minimal singularity in the family of $F_{(\lambda)}(\rho; W)$. In fact, $F_{(0)}(\rho; W)$ is nonsingular. For $\mu = 1/2$, all functions of the family $F_{(\lambda)}(\rho; W)$ have the same type of asymptotics: $F_{(\lambda)}(\rho; W) = O(1)$ as $\rho \to 0$.

We obtain the same results for the spectrum and complete orthonormalized set of the eigenvectors in the case $\lambda = -\pi/2$.

II. In the same manner, if $\lambda = 0$, we obtain that $F_{(0)}(\rho; W) = m_e^{\varkappa_0} F_2(\rho; W)$; the simple spectrum of $\hat{h}_0\,(s, l_0)$ is given by

$$\operatorname{spec} \hat{h}_0\,(s, l_0) = \{E_{\mathfrak{n}}(0),\ \mathfrak{n} \in \mathcal{Z}\},\ \mathcal{Z} = \left\{n_\zeta \in \zeta\mathbb{Z}_+,\ \zeta = \pm\right\},$$

and

$$\sigma'(E) = \sum_{\mathfrak{n}\in\mathcal{Z}} m_e^{-2\varkappa_0} Q_{0|\mathfrak{n}}^2 \delta(E - E_{\mathfrak{n}}(0)),$$

$$Q_{0|\mathfrak{n}} = \sqrt{\frac{(\gamma/2)^\mu\,\Gamma(|\mathfrak{n}| + \mu)(1 - sME_{\mathfrak{n}}^{-1}(0))}{|\mathfrak{n}|!\Gamma^2(\mu)}}\,,$$

where $E_{0|\mathfrak{n}}$ are solutions of the equation

$$\alpha_2 = \mu - \left(E_{\mathfrak{n}}^2(0) - M^2\right)/2\gamma = -|\mathfrak{n}|,\ E_{\mathfrak{n}}(0) = \zeta M_{|\mathfrak{n}|+\mu},$$

and $n_+ = 0$ and $n_- = 0$ are considered different elements of $\mathcal{Z}$.

The eigenvectors $\overset{III}{U}_{0|\mathfrak{n}} = \overset{III}{U}_{0|\mathfrak{n}}\,(0, s, l_0, p_z; \rho) = Q_{0|\mathfrak{n}} F_2(\rho; E_{\mathfrak{n}}(0))$, $\mathfrak{n} \in \mathcal{Z}$, of the Hamiltonian $\hat{h}_0\,(s, l_0)$ form a complete orthonormalized system in the space $\mathbb{L}^2(\mathbb{R}_+)$ of doublets $F\,(\rho)$.

We note that the spectrum, spectral function, and eigenfunctions of $\hat{h}_0\,(s, l_0)$ can be obtained from the respective expressions for the second region, $\varkappa_l \geq 1/2$, by the substitution $l = 0$. We also recall that for $\mu > 1/2$, the function $F_{(0)}(\rho; W) = m_e^{\varkappa_0} F_2(\rho; W)$ has a minimal singularity at the origin in the family of functions $F_{(\lambda)}(\rho; W)$; in fact, $F_{(0)}(\rho; W)$ is completely nonsingular.

III. Now we consider the general case $|\lambda| < \pi/2$. In this case we can equivalently write

$$\sigma'(E) = -\left(\pi\cos^2\lambda\right)^{-1} \operatorname{Im}\omega^{-1}(E + i0) = \sum_{k\in\mathbb{Z}} Q_k^2 \delta(E - E_k(\lambda)),$$

$$\omega(W) = t(W) + \tan\lambda,\ \omega'(E_k(\lambda)) > 0,\ Q_k = \left[\sqrt{\omega'(E_k(\lambda))}\cos\lambda\right]^{-1},$$

$$t(W) = \kappa\frac{(W + sM)\Gamma(-w/2\gamma)}{m_e\Gamma(\mu - w/2\gamma)},\ \kappa = \frac{\left(2m_e^2/\gamma\right)^\mu\,\Gamma(\mu)}{2\Gamma(1-\mu)} > 0,$$

$$t(E_k(\lambda)) = -\tan\lambda,\ t'(E_k(\lambda)) > 0,\ \partial_\lambda E_k(\lambda) = -\left[t'(E_k(\lambda))\cos^2\lambda\right]^{-1} < 0.$$

The function

$$t(E) = \kappa m_e^{-1}\Gamma^{-1}(\mu - w/2\gamma)(E + sM)\Gamma(-w/2\gamma)$$

has the properties: $t(\mathcal{E}_{\mathfrak{n}(s)} \pm 0) = \mp\infty$; $t(E_{\mathfrak{n}}(0)) = 0$. Thus, we obtain the following:

(a) $s = 1$.
In each interval $(\mathcal{E}_{n_- -1}, \mathcal{E}_{n_-})$, $n_- \leq -1$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue $E_{n_-}(\lambda)$ that increases monotonically from $\mathcal{E}_{n_- -1} + 0$ (passing $E_{n_-}(0)$) to $\mathcal{E}_{n_-} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$; in the interval $(\mathcal{E}_{-1}, \mathcal{E}_{n_+=0})$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue $E_{n_-=0}(\lambda)$ that increases monotonically from $\mathcal{E}_{-1} + 0$ (passing $E_{n_-=0}(0)$) to $\mathcal{E}_{n_+=0} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$; in each interval $(\mathcal{E}_{n_+}, \mathcal{E}_{n_+ +1})$, $n_+ \geq 0$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue $E_{n_+}(\lambda)$ that increases monotonically from $\mathcal{E}_{n_+} + 0$ (passing $E_{n_+}(0)$) to $\mathcal{E}_{n_+ +1} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$.

(b) $s = -1$.
In each interval $(\mathcal{E}_{n_- -1}, \mathcal{E}_{n_-})$, $n_- \leq 0$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue $E_{n_-}(\lambda)$ that increases monotonically from $\mathcal{E}_{n_- -1} + 0$ (passing $E_{n_-}(0)$) to $\mathcal{E}_{n_-} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$; in the interval $(\mathcal{E}_{n_-=0}, \mathcal{E}_{n_+=1})$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue $E_{n_+=0}(\lambda)$ which increases monotonically from $\mathcal{E}_{n_-=0} + 0$ (passing $E_{n_-=0}(0)$) to $\mathcal{E}_{n_+=1} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$; in each interval $(\mathcal{E}_{n_+}, \mathcal{E}_{n_+ +1})$, $n_+ \geq 1$, for a fixed $\lambda \in (-\pi/2, \pi/2)$, there exists an eigenvalue E_{n_+} that increases monotonically from $\mathcal{E}_{n_+} + 0$ (passing $E_{n_+}(0)$) to $\mathcal{E}_{n_+ +1} - 0$ as λ goes from $\pi/2 - 0$ (passing 0) to $-\pi/2 + 0$.

10.4 Summary

In the previous subsubsections, we have constructed all s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(s, l, p_z)$ as s.a. extensions of the symmetric operators $\hat{h}(s, l, p_z)$ for any s, l, and p_z and for any values of ϕ_0, μ, and γ. The complete s.a. Dirac operators $\hat{H}_{\mathfrak{e}}$ associated with the Dirac differential operation $\check{H}$ are constructed from the sets of $\hat{h}_{\mathfrak{e}}(s, l, p_z)$ by means of a procedure of "direct summation over s and l and direct integration over p_z". Each set of possible s.a. radial Hamiltonians $\hat{h}_{\mathfrak{e}}(s, l, p_z)$ generates a translationary and rotationally invariant[8] s.a. Hamiltonian $\hat{H}_{\mathfrak{e}}$. Namely, let $\mathbb{G}$ be the group of the above space transformations $S : \mathbf{r} \longmapsto S\mathbf{r}$. This group is unitarily represented in $\mathfrak{H}$: if $S \in \mathbb{G}$, then the corresponding operator U_S is defined by

$$(U_S\,\psi)(\mathbf{r}) = \mathrm{e}^{-i\theta\Sigma^3/2}\psi(S^{-1}\mathbf{r}),\ \forall\psi \in \mathfrak{H},$$

where θ is the rotation angle of the vector **æ** around the z-axis. The operator $\hat{H}$ evidently commutes with U_S for any S. We consider only such s.a. extensions

[8]That is, invariant under rotations around the z-axis and under translations along the z-axis.

$\hat{H}_{\mathfrak{e}}$ of $\hat{H}$ that also commute with U_S for any S. This condition is the explicit form of the invariance, or symmetry, of a quantum Hamiltonian under the space transformations. As in classical mechanics, this symmetry allows a separation of the cylindrical coordinates ρ, φ, and z and a reduction of the three-dimensional problem to a one-dimensional radial problem. Let V be a unitary operator defined by the relationship

$$(Vf)(\rho,\varphi,z) = \frac{1}{2\pi\sqrt{\rho}}\int_{\mathbb{R}_z} \mathrm{d}p_z \sum_{l\in\mathbb{Z}} \mathrm{e}^{ip_z z}\Big[S_l(\varphi)F(s,l,p_z,\rho)\Big] \otimes e_s(p_z),$$

where $S_l(\varphi)$ and $e_s(p_z)$ are given respectively by (10.38) and (10.37).

Similarly to the considerations in Sects. 10.2.1 and 10.2.2, it is natural to expect that any s.a. Hamiltonian $\hat{H}_{\mathfrak{e}}$ can be represented in the form

$$\hat{H}_{\mathfrak{e}} = V\int_{\mathbb{R}_z} \mathrm{d}p_z \sum_{s=\pm 1}\sum_{l\in\mathbb{Z}} \hat{h}_{\mathfrak{e}}(s,l,p_z)V^{-1},$$

where $\hat{h}_{\mathfrak{e}}(s,l,p_z)$ for fixed s, l, and p_z is an s.a. extension of symmetric operator $\hat{h}(s,l,p_z)$ associated with the differential operation $\check{h}(s,l,p_z)$ given by (10.40). The operator $\hat{h}(s,l,p_z)$ is defined on the domain $D_{h(s,l,p_z)} = \mathcal{D}(\mathbb{R}_+) \subset \mathbb{L}^2(\mathbb{R}_+,\mathrm{d}\rho)$ in the Hilbert space $\mathbb{L}^2(\mathbb{R}_+,\mathrm{d}\rho)$ of functions $F(\rho,l,p_z)$ with the scalar product

$$(F_1(s,l,p_z),F_2(s,l,p_z)) = \int_{\mathbb{R}_+} \overline{F_1(s,l,p_z,\rho)}F_2(s,l,p_z,\rho)\mathrm{d}\rho.$$

An exact expression for $\hat{H}_{\mathfrak{e}}$ is

$$\hat{H}_{\mathfrak{e}} = V\int_{\mathbb{R}_z}^{\oplus} \mathrm{d}p_z \sum_{s=\pm 1}^{\oplus}\sum_{l\in\mathbb{Z}}^{\oplus} \hat{h}_{\mathfrak{e}}(s,l,p_z)V^{-1}.$$

Its rigorous justification is discussed in [78].

The inversion formulas in Hilbert space $\mathfrak{H}$ are correspondingly obtained from the known radial inversion formulas by a procedure of summation over s,l, and integration over p_z. It should be noted that here we must consider the extension parameter λ a function of s and p_z, $\lambda = \lambda(s,p_z)$. In what follows, $\int \mathrm{d}p_z$ means $\int_{-\infty}^{\infty} \mathrm{d}p_z$.

Thus, we can summarize as follows: For $\mu = 0$, there is a unique s.a. Dirac operator $\hat{H}_{\mathfrak{e}}$. Its spectrum is simple and given by

$$\operatorname{spec}\hat{H}_{\mathfrak{e}} = (-\infty,-m_e] \cup [m_e,\infty).$$

The generalized eigenfunctions $\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r})$ of $\hat{H}_{\mathfrak{e}}$,

$$\begin{aligned}
\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}) &= \frac{1}{2\pi\sqrt{\rho}} e^{ip_z z} S_l(\varphi) F_{\mathfrak{n}(s)}(s,l,p_z;\rho) \otimes e_s(p_z), \\
F_{\mathfrak{n}(s)}(s,l,p_z;\rho) &= \begin{cases} \overset{I}{U}_{\mathfrak{n}(s)}(s,l,p_z;\rho), & l \le 0 \\ \overset{II}{U}_{\mathfrak{n}(s)}(s,l,p_z;\rho), & 1 \le l \le |\mathfrak{n}(s)| \end{cases}, \\
\check{H}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}) &= E_{s,p_z,\mathfrak{n}(s),l}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}), \\
E_{s,p_z,\mathfrak{n}(s),l} &= \zeta\sqrt{m_e^2 + p_z^2 + 2\gamma\,|\mathfrak{n}(s)|},\ \mathfrak{n}(s) \in \mathcal{Z}(s),\ l \le |\mathfrak{n}(s)|,
\end{aligned}$$

where $\mathcal{Z}(s)$ is defined by (10.55), and doublets $\overset{I}{U}_{\mathfrak{n}(s)}(s,l,p_z;\rho)$ and $\overset{II}{U}_{\mathfrak{n}(s)}(s,l,p_z;\rho)$ are given respectively by (10.56) and (10.59), form a complete orthonormalized system in the Hilbert space $\boldsymbol{L}^2(\mathbb{R}^3)$ of Dirac spinors. The latter means that we have the following inversion formulas:

$$\begin{aligned}
\Psi(\mathbf{r}) &= \int dp_z \sum_{s=\pm 1} \sum_{\mathfrak{n}(s)\in\mathcal{Z}(s)} \sum_{l\le|\mathfrak{n}(s)|} \Phi_{s,p_z,\mathfrak{n}(s),l}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}), \\
\Phi_{s,p_z,\mathfrak{n}(s),l} &= \int \overline{\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r})}\Psi(\mathbf{r})d\mathbf{r}, \\
\int |\Psi(\mathbf{r})|^2 d\mathbf{r} &= \int dp_z \sum_{s=\pm 1} \sum_{\mathfrak{n}(s)\in\mathcal{Z}(s)} \sum_{l\le|\mathfrak{n}(s)|} |\Phi_{s,l,p_z,n}|^2,\ \forall\Psi \in \boldsymbol{L}^2(\mathbb{R}^3).
\end{aligned}$$

We note that for $\lambda = 0$ and $\pm\pi/2$, the spectrum at $l = 0$ can be found explicitly; see the third region in Sect. 10.3.3.

For $\mu > 0$, there is a family of s.a. Dirac operators $\hat{H}_{\{\lambda(s,p_z)\}}$ parameterized by two real-valued functions $\lambda(s,p_z)$, $\lambda \in \mathbb{S}(-\pi/2,\pi/2), s = \pm 1$. Their spectra are degenerate and continuous.

A complete set of generalized eigenfunctions of $\hat{H}_{\{\lambda(s,p_z)\}}$ consists of $\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r})$ and $\Psi^{\lambda(s,p_z)}_{s,p_z,k,l_0}(\mathbf{r})$. These bispinors have the form

$$\begin{aligned}
\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}) &= \frac{1}{2\pi\sqrt{\rho}} e^{ip_z z} S_l(\varphi) F_{\mathfrak{n}(s)}(s,l,p_z;\rho) \otimes e_s(p_z), \\
F_n(s,l,p_z;\rho) &= \begin{cases} \overset{I}{U}_n(s,l,p_z;\rho), & l \le -1, \\ \overset{II}{U}_n(s,l,p_z;\rho), & 1 \le l \le |\mathfrak{n}(s)|, \end{cases} \\
&\mathfrak{n}(s) \in \mathcal{Z}(s),\ l \le |\mathfrak{n}(s)|,\ l \ne 0,
\end{aligned}$$

and

$$\Psi_{s,p_z,k,l_0}^{\lambda(s,p_z)}(\mathbf{r}) = \frac{1}{2\pi\sqrt{\rho}} \mathrm{e}^{ip_z z} S_{l_0}(\varphi) \overset{III}{U_k}(\lambda(s,p_z), s, p_z; \rho) \otimes e_s(p_z),\ k \in \mathbb{Z},$$

where $\overset{III}{U_n}(\lambda(s,p_z), s, p_z; \rho)$ are given by (10.63) with the substitution $\lambda(s) \to \lambda(s, p_z)$, so that

$$\begin{aligned}
\check{H}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}) &= E_{s,p_z,\mathfrak{n}(s),l}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r}),\ l \le |\mathfrak{n}(s)|,\ l \neq 0,\\
E_{s,p_z,\mathfrak{n}(s),l} &= \sigma\sqrt{m_e^2 + p_z^2 + 2\gamma[|\mathfrak{n}(s)| + \theta(l)]},\ \theta(l)\\
&= \begin{cases} 0, & l \le 0, \\ 1, & l \ge 1, \end{cases}\\
\check{H}\Psi_{s,p_z,k,l_0}^{\lambda(s,p_z)}(\mathbf{r}) &= E_{s,p_z,k,l_0}^{\lambda(s,p_z)}\Psi_{s,p_z,k,l_0}^{\lambda(s,p_z)}(\mathbf{r}),\\
E_{s,p_z,k,l_0}^{\lambda(s,p_z)} : \Omega\left(\lambda, E_{s,p_z,k,l_0}^{\lambda}\right) &= 0, \quad \Omega(\lambda, W) = \frac{\cos\lambda + a(W)\sin\lambda}{\sin\lambda - a(W)\cos\lambda},\\
a(W) &= \frac{2m_e^{2\mu-1}(\gamma/2)^{1-\mu}\,\Gamma(\mu)\,\Gamma(1-\mu-w/2\gamma)}{(W+sM)\,\Gamma(1-\mu)\,\Gamma(-w/2\gamma)}\,.
\end{aligned}$$

In the case under consideration, the corresponding inversion formulas have the form

$$\begin{aligned}
\Psi(\mathbf{r}) = \int \mathrm{d}p_z \sum_{s=\pm 1}\Bigg[&\sum_{\mathfrak{n}(s)\in\mathcal{Z}(s)}\ \sum_{l\le|\mathfrak{n}(s)|,l\neq 0} \Phi_{s,p_z,\mathfrak{n}(s),l}\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r})\\
&+ \sum_k \Phi_{s,p_z,k,l_0}\Psi_{s,p_z,k,l_0}^{\lambda(s,p_z)}(\mathbf{r})\Bigg],\ \forall\Psi \in \boldsymbol{L}^2\left(\mathbb{R}^3\right),
\end{aligned}$$

$$\begin{aligned}
\Phi_{s,p_z,\mathfrak{n}(s),l} &= \int \overline{\Psi_{s,p_z,\mathfrak{n}(s),l}(\mathbf{r})}\Psi(\mathbf{r})\mathrm{d}\mathbf{r},\ l \neq 0,\\
\Phi_{s,p_z,k,l_0} &= \int \overline{\Psi_{s,p_z,k,l_0}^{\lambda(s,p_z)}(\mathbf{r})}\Psi(\mathbf{r})\mathrm{d}\mathbf{r},
\end{aligned}$$

$$\int |\Psi(\mathbf{r})|^2\,\mathrm{d}\mathbf{r} = \int \mathrm{d}p_z \sum_{s=\pm 1}\left[\sum_{\mathfrak{n}(s)\in\mathcal{Z}(s)}\ \sum_{l\le|\mathfrak{n}(s)|,l\neq 0}\left|\Phi_{s,p_z,\mathfrak{n}(s),l}\right|^2 + \sum_k\left|\Phi_{s,p_z,k,l_0}\right|^2\right].$$

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Notation

- a.c. : absolutely continuous
- a.b. conditions : asymptotic boundary conditions
- AB : Aharonov–Bohm
- iff : if and only if
- MSF : magnetic-solenoid field
- QM : quantum mechanics, or quantum-mechanical, and so on
- s.a. : self-adjoint
- $\mathrm{diag}(a,b) = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$, $\mathrm{antidiag}(a,b) = \begin{pmatrix} 0 & b \\ a & 0 \end{pmatrix}$
- $F = \begin{pmatrix} f \\ g \end{pmatrix} = (f \diagup g)$, this notation is used for two-component columns, spinors, and doublets
- $\mathbb{C}^{\infty}(a,b)$: the linear space of smooth (infinitely differentiable) functions on the interval (a,b)
- $D(a,b)$: space of arbitrary functions with compact support on the interval (a,b)
- $D_r(a,b)$: space of arbitrary functions on the interval (a,b) with support bounded from the right
- $D_l(a,b)$: space of arbitrary functions on the interval (a,b) with support bounded from the left
- $\mathcal{D}(a,b)$: linear complex space of smooth compactly supported functions on an interval (a,b)
- $\mathcal{D}_R(a,b)$: linear space of real smooth compactly supported functions on the interval (a,b)
- $\mathcal{D}\left(\mathring{\mathbb{R}}\right) = \mathcal{D}(-\infty,0) \cup \mathcal{D}(0,\infty)$
- $L^2(a,b)$: space of functions square-integrable on (a,b)
- $\mathbb{L}^2(\mathbb{R}_+) = L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$: space of two-component columns (doublets) square-integrable on the semiaxis
- $\boldsymbol{L}^2\left(\mathbb{R}^3\right) = \sum\nolimits_{\alpha=1}^{\oplus 4} \mathfrak{H}_\alpha, \mathfrak{H}_\alpha = L^2\left(\mathbb{R}^3\right)$: space of Dirac spinors square-integrable on $\mathbb{R}^3$

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- $D^*_{\check{f}}(a,b)$: the natural domain for a s.a. differential operation $\check{f}$ defined on an interval (a,b)
- $\tilde{O}(x) = 1 + O(x)$
- I is the 2×2 identity matrix and $\mathbb{I}$ is the 4×4 identity matrix
- $\mathbb{N} = \{1, 2, \dots\}$: the set of natural numbers
- $\mathbb{Z} = \{0, \pm 1, \dots\}$: the set of integers
- $\mathbb{Z}_+ = \{0, 1, 2, \dots\}$: the set of nonnegative integers
- $\mathbb{Z}_- = \{0, -1, -2, \dots\}$: the set of nonpositive integers
- $\mathcal{N}_\zeta = \begin{cases} \mathbb{N}, \ \zeta = 1 \\ \mathbb{Z}_+, \ \zeta = -1 \end{cases}$
- $\mathbb{R} = (-\infty, \infty)$: the set of all real numbers, the real axis
- $\mathbb{R}_+ = [0, \infty)$: the set of nonnegative real numbers, semiaxis
- $\mathbb{R}_- = (-\infty, 0]$: the set of nonpositive real numbers
- $\mathbb{R}^n$: n-dimensional real linear space, the set of all real n-tuples $(x^1, \dots, x^n)$
- $\mathring{\mathbb{R}} = (-\infty, 0) \cup (0, \infty)$
- $\overline{\mathbb{R}}$: the compactified real axis where $-\infty$ and ∞ are identified: $\overline{\mathbb{R}} = \{\lambda : -\infty \le \lambda \le \infty, \ -\infty \sim \infty\}$; $\overline{\mathbb{R}}$ is homeomorphic to a circle.
- $\mathbb{S}(a,b) = [a,b], a \sim b$; $\mathbb{S}(a,b)$ is homeomorphic to a circle
- $\mathbb{C} = \{z = x + iy : x, y \in \mathbb{R}\}$: the set of all complex numbers, the complex plane
- $\mathbb{C}_+ = \{z = x + iy : x, y \in \mathbb{R}, \ y > 0\}$: the set of complex numbers with positive imaginary part
- $\mathbb{C}_- = \{z = x + iy : x, y \in \mathbb{R}, \ y < 0\}$: the set of complex numbers with negative imaginary part
- $\mathbb{C}' = \{z = x + iy : x, y \in \mathbb{R}, \ y \neq 0\} = \mathbb{C}_+ \cup \mathbb{C}_-$: the set of complex numbers with nonzero imaginary parts
- regp $\hat{f}$: the resolvent set of an operator $\hat{f}$
- spec $\hat{f}$: the spectrum of an operator $\hat{f}$
- $\check{K}_x^{[k]}$: the quasiderivative of order k with respect to x
- $\hat{f}(z) = \hat{f} - z\hat{I}_{D_f}$
- $\hat{\mathcal{R}}(z) = \left(\hat{f}(z)\right)^{-1}$, $\hat{\mathcal{R}}(z)$ is called the resolvent if z belongs to the resolvent set
- $\mathrm{Wr}(u_1, \dots, u_m)$: the Wronskian of the set of functions $u_1, \dots, u_m$;

$$\mathrm{Wr}(u_1, \dots, u_m) = \det \|W_{ki}\|, \ W_{ki} = u_i^{(k-1)}(x), \ k, i = 1, \dots, m.$$

- $\mathbb{W}\mathrm{r}(u_1, \dots, u_m)$: the quasi-Wronskian of the set of functions $u_1, \dots, u_m$;

$$\mathbb{W}\mathrm{r}(u_1, \dots, u_m) = \det \|\mathbb{W}_{ki}\|, \ \mathbb{W}_{ki} = u_i^{[k-1]}(x), \ k, i = 1, \dots, m.$$

- An overline denotes complex conjugation unless otherwise specified
- The derivative of order k in x of a function $\psi(x)$ is commonly denoted by $\psi^{(k)}(x)$. In addition, we also use the following notation:

$$d_x = \mathrm{d}/\mathrm{d}x, \ d_x f(x) = f'(x), \dots, \ d_x^n f(x) = f^{(n)}(x).$$

- The following notation is adopted for special functions (this notation is in agreement with that used in the reference book [81]): $J_\mu(x)$ is the Bessel function of the first kind; $H_\nu^{(1)}(x)$ is the first Hankel function; $I_\mu(x)$ is the Bessel function of imaginary argument; $K_\mu(x)$ is the MacDonald function (the first Hankel function of imaginary argument); $\Phi(\alpha, \beta; x)$ and $\Psi(\alpha, \beta; x)$ are the confluent hypergeometric functions; $F(\alpha, \beta; \gamma; x)$ is the Gauss hypergeometric function; $H_n(x)$ are the Hermite polynomials; $\psi(x)$ is the logarithmic derivative of the Γ-function, $\psi(x) = \Gamma'(x)\Gamma^{-1}(x)$
- $\mathbf{C} = 0.5772156649\ldots$: Euler's constant
- In Chaps. 9 and 10, in which relativistic systems are considered, Greek vector and tensor indices take on the values 0, 1, 2, 3 and Latin indices take on the values 1, 2, 3 unless otherwise specified; the convention about summation over repeated indices is adopted unless otherwise specified; the metric in the four-dimensional flat space–time is determined by the Minkowski tensor $\eta_{\mu\nu} = \mathrm{diag}\,(1, -1, -1, -1)$; contravariant vectors are represented as

$$(a^\mu) = \left(a^0, \mathbf{a}\right) = \left(a^0, a^i\right),\ a^1 = a_x,\ a^2 = a_y,\ a^3 = a_z,$$

the space–time coordinates are denoted by

$$x = (x^\mu) = \left(x^0, \mathbf{r}\right) = \left(x^0, x^i\right) = (t, \mathbf{r}),\ \mathrm{d}x = \mathrm{d}x^0\mathrm{d}\mathbf{r},$$
$$x^1 = x,\ x^2 = y,\ x^3 = z,\ \mathrm{d}\mathbf{r} = \mathrm{d}x^1\mathrm{d}x^2\mathrm{d}x^3,$$

and

$$\partial A/\partial x^\mu = \partial_\mu A,\ \partial/\partial t = \partial_t = \partial_0,\ \partial_1 = \partial_x,\ \partial_2 = \partial_y,\ \partial_3 = \partial_z$$

- $F(x)|_a^b = \lim\limits_{x\to b} F(x) - \lim\limits_{x\to a} F(x)$

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