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Solvable Models in Quantum Mechanics

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"La filosofia è scritta in questo grandissimo libro che continuamente ci sta aperto innanzi a gli occhi (io dico l'universo), ma non si può intendere se prima non s'impara a intender la lingua, e conoscer i caràtteri, ne' quali è scritto. Egli è scritto in lingua matematica, e i caràtteri son triangoli, cerchi, ed altre figure geometriche, senza i quali mezi è impossibile a intenderne umanamente parola; senza questi è un aggirarsi vanamente per un oscuro laberinto."

Galileo Galilei, p. 38 in *Il Saggiatore*, Ed. L. Sosio, Feltrinelli, Milano (1965)

"Philosophy is written in this grand book—I mean the universe—which stands continually open to our gaze, but it cannot be understood unless one first learns to comprehend the language and to interpret the characters in which it is written. It is written in the language of mathematics, and its characters are triangles, circles, and other geometrical figures, without which it is humanly impossible to understand a single word of it; without these, one is wandering about in a dark labyrinth."

Galileo Galilei, in *The Assayer* (transl. from Italian by S. Drake, pp. 106–107 in L. Geymonat, *Galileo Galilei*, McGraw-Hill, New York (1965))

Preface

Solvable models play an important role in the mathematical modeling of natural phenomena. They make it possible to grasp essential features of the phenomena and to guide the search for suitable methods of handling more complicated and realistic situations.

In this monograph we present a detailed study of a class of solvable models in quantum mechanics. These models describe the motion of a particle in a potential having support at the positions of a discrete (finite or infinite) set of point sources. We discuss both situations in which the strengths of the sources and their locations are precisely known and the cases where these are only known with a given probability distribution. The models are solvable in the sense that their resolvents and associated mathematical and physical quantities like the spectrum, the corresponding eigenfunctions, resonances, and scattering quantities can be determined explicitly.

There is a large literature on such models which are called, because of the interactions involved, by various names such as, e.g., "point interactions," "zero-range potentials," "delta interactions," "Fermi pseudopotentials," "contact interactions." Their main uses are in solid state physics (e.g., the Kronig–Penney model of a crystal), atomic and nuclear physics (describing short-range nuclear forces or low-energy phenomena), and electromagnetism (propagation in dielectric media).

The main purpose of this monograph is to present in a systematic way the mathematical approach to these models, developed in recent years, and to illustrate its connections with previous heuristic derivations and computations. Results obtained by different methods in disparate contexts are unified in this way and a systematic control on approximations to the models, in which the point interactions are replaced by more regular ones, is provided.

There are a few happy cases in mathematical physics in which one can find solvable models rich enough to contain essential features of the phenomena to be studied, and to serve as a starting point for gaining control of general situations by suitable approximations. We hope this monograph will convince the reader that point interactions provide such basic models in quantum mechanics which can be added to the standard ones of the harmonic oscillator and the hydrogen atom.

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Contents

Introduction

In this monograph we present a detailed investigation of a class of solvable models of quantum mechanics; namely, models given by a Schrödinger Hamiltonian with potential supported on a discrete (finite or infinite) set of points ("sources"). Such point interaction models are "solvable" in the sense that their resolvents can be given explicitly in terms of the interaction strengths and the location of the sources. As a consequence the spectrum, the eigenfunctions, as well as resonances and scattering quantities, can also be determined explicitly. Models of this type have already been discussed extensively, particularly in the physical literature concerned with problems in atomic, nuclear, and solid state physics. Our main purpose with this monograph is to provide a unifying mathematical framework for a large body of knowledge which has been accumulated over decades in different fields, often by heuristic considerations and numerical computations, and often without knowledge of detailed results in other fields. Moreover, we systematically expose advances in the study of point interaction models obtained in recent years by a more mathematically minded approach. In this introduction we would briefly like to introduce the subject and its history, as well as to illustrate the content of our monograph. Furthermore, a few related topics not treated in this monograph will be mentioned with appropriate references.

The main basic quantum mechanical systems we discuss are heuristically given (in suitable units and coordinates) by "one particle, many center Hamiltonians" of the form

$$H = -\Delta + \sum_{y \in Y} \lambda_y \delta_y(\cdot), \tag{1}$$

where Δ denotes the self-adjoint Laplacian in $L^2(\mathbb{R}^d)$ with domain $H^{2,2}(\mathbb{R}^d)$. Here $d = 1, 2, 3$ is the dimension of the underlying configuration space, Y is a discrete (finite or countably infinite) subset of $\mathbb{R}^d$, λ_y is a coupling constant attached to the point source located at y, and δ_y is the Dirac δ-function at y (i.e., the unit measure concentrated at y). The quantum mechanical particle thus moves under the influence of a "contact potential" created by "point sources" of strengths λ_y located at y. The basic idea behind the study of such models is that, once their Hamiltonians have been well defined and understood, they can serve as corner stones for more complicated and more realistic interactions, obtained by various perturbations, approximations, and extensions of (1). Models with interactions of type (1) occur in the literature under various names, like "point interaction models," "zero-range potential models," "delta interaction models," "Fermi pseudopotential models," and "contact interaction models."

Historically, the first influential paper on models of type (1) was that by Kronig and Penney [307], in 1931, who treated the case $d = 1$ and $Y = \mathbb{Z}$ with $\lambda_y = \lambda$ independent of y. This "Kronig–Penney model" has become a standard reference model in solid state physics, see, e.g., [290], [493]. It provides a simple model for a nonrelativistic electron moving in a fixed crystal lattice. A few years later, Bethe and Peierls [86] (1935) and Thomas [485] (1935) started to discuss models of type (1) for $d = 3$ and $Y = \{0\}$, in order to describe the interaction of a nonrelativistic quantum mechanical particle interacting via a "very short range" (in fact zero range) potential with a fixed source. By introducing the center of mass and relative coordinates this can also be looked upon as a model of a deuteron with idealized zero-range nuclear force between the nucleons. In particular, Thomas realized that a renormalization of the coupling constant is necessary (see below) and exhibited an approximation of the Hamiltonian (1) in terms of local, scaled short-range potentials. His paper was quite influential and was the starting point for investigations into corresponding models in the case of a triton (three particles interacting by two-body zero-range potentials). It soon turned out that in the triton case the naively computed binding energy is actually infinite, so that the heuristically defined Hamiltonian is unbounded from below and hence physically not acceptable, see, e.g., [134], [135], [441], [485].

Subsequent studies aimed at the clarification of this state of affairs led in particular to the first rigorous mathematical work by Berezin and Faddeev [81] in 1961 on the definition of Hamiltonians of type (1) for $d = 3$ as self-adjoint operators in $L^2(\mathbb{R}^3)$. Let us shortly describe the actual mathematical problem involved in the case where Y consists of only one point y. Any possible mathematical definition of a self-adjoint operator H of the heuristic form $-\Delta + \lambda\delta_y$ in $L^2(\mathbb{R}^d)$ should take into account the fact that, on the space $C_0^\infty(\mathbb{R}^d - \{y\})$ of smooth functions which vanish outside a compact subset of the complement of $\{y\}$ in $\mathbb{R}^d$, H should coincide with $-\Delta$. For $d \geq 4$ this already forces H to be equal to $-\Delta$ on $H^{2,2}(\mathbb{R}^d)$ since $-\Delta|_{C_0^\infty(\mathbb{R}^d - \{y\})}$ is essentially self-adjoint for $d \geq 4$ [389]. For $d = 2, 3$ it turns out that there is a one-parameter family of self-adjoint operators, indexed by a "renormalized coupling constant" α, all realizing the heuristic expression $-\Delta + \lambda\delta_y$. In physical terms, the coupling constant λ in the heuristic expression $-\Delta + \lambda\delta_y$ has to be "renormalized" and turns out to be of the form $\lambda = \eta + \alpha\eta^2$, with η infinitesimal and $\alpha \in (-\infty, \infty]$. This was put on a mathematical basis in [81] using Krein's theory of self-adjoint extensions (cf. Sect. I.1.1). Several other mathematical definitions of (1) appeared later in the literature, as will be discussed briefly below, but perhaps the most intuitive mathematical explanation nowadays is provided by nonstandard analysis. It should also be remarked that the necessity of renormalization for $d = 2, 3$ mentioned above is not tied to the interpretation of H as an operator, the same applies for H interpreted as a quadratic form. In particular, it is not possible, without renormalization, to decribe H as a perturbation of $-\Delta$ in the sense of quadratic forms [188]. This is in sharp contrast to the one-dimensional case which allows a straightforward description of δ-interactions by means of quadratic forms. Actually, a new phenomenon occurs in one dimension: Since (in contrast to $d = 2, 3$) $-\Delta|_{C_0^\infty(\mathbb{R}-\{y\})}$ exhibits a four-parameter family of self-adjoint extensions in $L^2(\mathbb{R})$, additional types of point interactions (e.g., δ'-interactions, cf. Ch. I.4) exist.

But let us close this short digression on the mathematical definition of (1) and return to the historical development of the subject. The investigations of Thomas and others in nuclear physics (starting in the 1930s), which we mentioned above, were persued in different directions during the following decades. In particular, Fermi [179] discussed by similar methods the motion of neutrons in hydrogeneous substances, introducing the so-called Fermi pseudopotential made explicit by Breit [110] 10 years later (the Fermi pseudopotentials can be identified with point interactions for $d \leq 3$ [229]). Some of this work has now been incorporated into standard reference books on nuclear physics, see, e.g., [93].

Somewhat parallel to this work, models involving zero-range potentials began to be studied in the 1950s in connection with many-body theories and quantum statistical mechanics. Here, particular attention was paid to obtaining results on certain statistical quantities by using explicit computations and various approximations, the point interactions being used as limit cases around which one could reach more realistic models by perturbation theory. For this work we shall give references below.

Let us mention yet another area of physics in which problems arise and which are essentially equivalent to those of many-body Hamiltonians with two-body point interactions. This is the theory of sound and electromagnetic wave propagations in dielectric media, where the role of the point interactions is replaced by boundary conditions at suitable geometric configurations. In the one-dimensional case ($d = 1$), such relations have been pointed out and exploited in the work by Heisenberg, Jost [275], Lieb and Koppe [323], Nussenzveig [366], and others. The book by Gaudin [194] contains many references to this subject. In the three-dimensional case ($d = 3$), the relation between Hamiltonians of type (1) and problems of electromagnetism (and acoustics) has not yet been exploited sufficiently; see, however, [228], [229],

[503] for recent developments (which are particularly interesting in connection with work on the construction of antennas).

We will now discuss the content of the monograph, and at the same time take the opportunity to make some complementary remarks. In each of the three parts, I to III, theorems and lemmas are numbered consecutively in the form $x \cdot y \cdot z$ where x refers to the chapter, y to the section and z to the number within the section. Equations are numbered in the same way. When we refer to equations, theorems, or lemmas from another part of the monograph, the appropriate roman number is added.

In this monograph we have divided the subject into three parts corresponding to point interactions with one center (Part I), finitely many centers (Part II) resp. infinitely many centers (Part III), according to whether Y consists of one, finitely many, or infinitely many points. Within the parts we separately discuss the three-dimensional case ($d = 3$) and the cases $d = 1, 2$. In the one-center problem (Part I) the first problem is to define the point interaction. Historically, the first discussions in the three-dimensional case go back to Bethe and Peierls [86] and Thomas [485], who used a characterization by boundary conditions (cf. Theorem I.1.1). We have already mentioned the approach by Berezin and Faddeev [81] using Krein's theory (for a similar discussion in the three-particle case, see [342], [343]). The modern approach by nonstandard analysis was developed in [12], [14], [37], [355]. Yet another approach, particularly suited to probabilistic interpretations, is the one by Dirichlet forms introduced by Albeverio, Høegh-Krohn, and Streit [32], [33]. Finally, let us mention various approaches based on constructing the resolvent by suitable limits of "regularized" resolvents [17], [24], [226]. These approaches also lead to results on convergence of eigenvalues, resonances, and scattering quantities (as we will discuss in Ch. I.1). Perturbations of the three-dimensional one-center problem by a Coulomb interaction is discussed in Ch. I.2. Here the historical origins may be found in the work of Rellich [392] in the 1940s; however, most results are quite recent with main contributions from Zorbas [512], Streit, and the authors [22].

Let us here mention some work we do not discuss in this monograph. It concerns time-dependent point interactions $-\Delta + \lambda(t)\delta(\cdot)$ and electromagnetic systems of the type $[-i\nabla - A(t)]^2 + \lambda\delta(\cdot)$ discussed in [111], [145], [146], [151], [239], [348], [349], [362], [405], [406], [472], [505], [506].

The one-center problem for a particle moving in one dimension is discussed in Ch. I.3 in the case of δ-interactions, and in Ch. I.4 in the case of δ'-interactions. In Ch. I.5 the case of a particle moving in two dimensions under the influence of a one-center point interaction is briefly discussed. The problems are similar to the three-dimensional case, however most results are based on recent work.

In Part II of this monograph we discuss Hamiltonians of type (1) with Y a finite subset of $\mathbb{R}^d$. In Ch. II.1 the three-dimensional case is treated. The methods of defining the Hamiltonian are similar to the methods introduced in Part I. In the physical literature, the model appears quite early and detailed results are derived heuristically, e.g., in [151], [277]. Mathematical studies started in the late 1970s [129], [226], [482], [483], [512]. In recent years a lot of work has gone into obtaining mathematical results concerning approximations, convergence of eigenvalues and resonances, and scattering theory on which we report in this chapter. Chapter II.2 (resp. II.3) report on detailed corresponding studies carried out recently on the one-dimensional case with δ- (resp. δ'-) interactions. Chapter II.4 reports on recent work on the two-dimensional case.

At this point we would like to mention a major subject which has been omitted from our monograph, namely, the case of multiparticle Hamiltonians, i.e., the case where (1) is replaced by

$$-\Delta + \sum_{i<j}^{N} \lambda_{ij}\delta(x_i - x_j), \tag{2}$$

where λ_{ij} are coupling constants for the δ-interactions between particles i and j at x_i resp. $x_j \in \mathbb{R}^d$. Such heuristic Hamiltonians describe a quantum mechanical N-particle system interacting via two-body point interactions ($-\Delta$ denotes the Nd-dimensional Laplacian). Our excuse for not including a discussion of this case is twofold. In the one-dimensional case (i.e., $d = 1$) the literature is very rich and a monograph by Gaudin [194] already exists (see also [83], [326]). Multiparticle problems with point interactions in one dimension have been studied extensively since the 1950s, particularly under the influence of work by Heisenberg on the scattering matrix for nuclear physics. Some early references are [9], [275], [323], [366], [498], [499], see also [326], [346] for some illustrations. More recent references, in addition to those given in [194], are [82], [113], [155], [156], [233], [310], [321], [328], [335], [338], [339], [340], [433], [449a], [468], [507].

In the two- and three-dimensional cases very few mathematical results are as yet available, despite considerable work carried out by physicists. We limit ourselves here to giving some hints to some studies in this area and some references. Flamand [184] gives a very good survey of work done on the three-particle problem ($N = 3$) in three dimensions ($d = 3$), up to 1967. This work was mainly carried out by physicists and mathematicians in the Soviet Union in connection with models of nuclear physics (triton and related models) [131], [134], [135], [150], [198], [224], [342], [343], [354], [364], [429], [441], [484], [485]. The main conclusion of this work is that a class of natural self-adjoint realizations of (2) are not bounded from below [342], [343]. However, the spectrum can be computed quite easily. In [34] a relation was observed between this problem and the so-called Efimov effect in three-particle systems with short-range, two-body potentials (i.e., the formation of infinitely many negative three-body bound states below zero, if at least two two-particle subsystems have a zero-energy resonance). Heuristically, the relation is brought about by a scaling argument. Two-dimensional multiparticle systems are discussed in [253], [327], [433].

Methodically related to the study of many-body systems is the study of quantum statistical mechanical systems, for which we shall also mention some references. Bose gases with hard-sphere interactions related to point interactions and Fermi pseudopotential models were discussed extensively in the 1950s, particularly by Huang, Luttinger, Wu, and Yang, see, e.g., [264], [265], [266], [320], [502]. Many-body systems of bosons with repulsive two-body δ-interactions were discussed by Lieb, Liniger, Yang, and coworkers, cf., e.g., [322], [324], [331], [508] and the references in [194], [326]. Fermions with two-body δ-interactions were studied by Lieb and others, see, e.g., [325] and the references in [194], [326].

Let us also mention that the heuristic nonrelativistic limit of quantum field theoretical models with ϕ_d^4-interaction is described by Schrödinger multiparticle Hamiltonians with two-particle δ-interactions in $d - 1$ dimensions. This is rigorously discussed for $d = 2$ in [154].

Let us now proceed to the description of work discussed in Part III of our monograph, treating point interactions with infinitely many centers. As we have mentioned already, a very influential model in solid state physics, discussed early in the literature, has been the Kronig–Penney model [307] (1931) in one dimension. An early heuristic treatment of a three-dimensional crystal with point interactions was given by Goldberger and Seitz [216] in 1947.

The systematic mathematical discussion of these and similar Hamiltonians in three dimensions is, however, much more recent and was started by the work of Grossmann, Mebkhout, and the present authors starting at the end of the 1970s. In general, Hamiltonians with infinitely many point interactions are defined as limits in the strong resolvent sense of Hamiltonians for N-point interactions as $N \to \infty$. In the case where the centers are periodically arranged, group-theoretical methods of reduction to simpler Hamiltonians, exploiting the symmetry, permit a more direct definition of the Hamiltonians. This leads to a particularly detailed treatment of spectral properties for the case of crystals ("Kronig–Penney"—or rather "Goldberger–Seitz"—type models in three dimensions) in Sect. III.1.4, as well as of embedded one- or two-dimensional lattices in $\mathbb{R}^3$, so-called "straight polymers" in Sect. III.1.5 resp. "monomolecular layers" in Sect. III.1.6. Some physical discussions of related systems are given in [151]. Scattering from half-crystals (Bragg scattering) is treated in Sect. III.1.7. This gives details on results announced earlier in [52]. The computation of Fermi surfaces for crystals is of basic importance in solid state physics. It is usually obtained by various approximations. The point interaction model gives the possibility of producing exact formulas for the Fermi surfaces as shown in Sect. III.1.8. This is based on work done by Høegh-Krohn, Holden, Johannesen, and Wentzel-Larsen [242]. We also discuss crystals with defects, as well as scattering from impurities in crystals in Sect. III.1.9.

In Ch. III.2 models with infinitely many δ-interactions in one dimension are discussed. Although the prototype of such models is the Kronig–Penney model already introduced in 1931, most mathematical results in this chapter have been obtained in recent years. The topics discussed in this chapter correspond to those treated in the three-dimensional case, Ch. III.1. In particular, Sect. III.2.3 treats the case of periodic δ-interactions, and Sect. III.2.4. develops spectral and scattering theory in connection with half-crystals. Quasi-periodic point interactions are briefly studied in Sect. III.2.5. The discussion of crystals with defects and impurity scattering in Sect. III.2.6 goes back originally to Saxon and Hutner [404].

In Ch. III.3 all the basic results of Ch. III.2 are extended to models with infinitely many δ'-interactions in one dimension. Let us remark at this point that in one dimension, δ'-interactions are nontrivial, in higher dimensions, $d \geq 2$, interactions supported on ν-dimensional hypersurfaces $0 \leq \nu \leq d - 1$ are nontrivial. For a discussion of point interactions on manifolds, see, e.g., [42], [125], [180], [226], [299], [424] and the references therein.

In Ch. III.4 we extend the results established for dimensions one and three to the two-dimensional case.

In Ch. III.5 we discuss random Hamiltonians with point interactions in one and three dimensions. Schrödinger operators with stochastic potentials have received a lot of attention in recent years, because of their importance as models for amorphous solids. Actually, at the end of the 1940s–early 1950s much work had already been done on one-dimensional models of disordered solids with point interactions. The paper by Saxon and Hutner [404] was very influential. It discussed, in particular, Schrödinger Hamiltonians with two types of atoms (binary alloys) characterized by coupling constants A and B conjecturing that gaps in the spectrum of both pure crystals (with pure atoms of type A (resp. B)) should also be present in arbitrary alloys (with random combination of A's and B's). It influenced other papers on the subject such as, e.g., [189] (see the extensive bibliography in [326] and in the notes in Ch. III.5) which treated a stochastic Poisson distribution of sources as an "impurity band" model or a "one-dimensional liquid metal" model. Incidentally, the relation with the one-dimensional version of a scalar–meson pair theory Hamiltonian, discussed by Montroll and Potts [344] in their study of interactions of lattice defects, was pointed out. Anderson, Mott, and others started in the 1950s to discuss, from the physical point of view, the phenomenon of localization, by which a discretized random Hamiltonian in three dimensions was conjectured to have a nonconducting phase at large disorder and a conducting phase at low disorder, the two phases being separated by a mobility edge. Mathematical work on the problem was originally started in the Soviet Union, see, e.g., [222], [223], [368]. Random point interactions were rigorously studied by Kirsch and Martinelli [286], [287], [288], [289] and the present authors [20], [30], [206] (our presentation in Ch. III.5 closely follows these papers). There are connections with work on the Laplacian with boundary conditions on small, randomly distributed spheres [181], [182], [183].

Let us also mention that random distributions of sources along Brownian paths have also been considered, both in the physical literature, e.g., [162], and in the mathematical literature [13], [14], as models for the motion of a quantum mechanical particle in the potential created by a polymer. There are applications, via a Feynman–Kac type formula, to the study of polymer measures of Edward's type [14], [162] and quantum field theory [14].

Appendices A–I give complements to the main text. Let us mention here that Appendix J treats Dirac Hamiltonians with point interactions in one dimension.

As a final note, we would like to mention that our monograph only discusses the class of solvable quantum mechanical models characterized by point interactions in $d \leq 3$ dimensions. Of course, there are many other solvable models in quantum mechanics. Their treatment would have made the size of this volume unmanageable, besides that the methods of solutions of these models are quite different from the ones we discuss here. In fact, their solvability relies on symmetries which allow a group-theoretical treatment (such models are often related to classically completely integrable systems). For a discussion of these topics, see, e.g., [10], [83], [185], [326], [367].

In the references we have tried to be as complete as possible; however, with the enormous number of publications over a wide range of fields, including mathematics, solid state physics, atomic and nuclear physics, and theoretical chemistry, we make no claim to being complete. The notes at the end of each chapter give some historical comments and references to the subject discussed.

For other presentations of some of the material discussed in this monograph we refer to the book by Demkov and Ostrovskii [151], and the survey papers [18], [20], [29], [454].

PART I

THE ONE-CENTER POINT INTERACTION

CHAPTER I.1

The One-Center Point Interaction in Three Dimensions

I.1.1 Basic Properties

In this section we develop a precise formulation for the point interaction (also called δ, or zero-range, or contact interaction or Fermi pseudopotential in the physics literature) centered at a fixed point y in three dimensions. Although our methods concentrate mainly on the concept of self-adjoint operator extensions, an alternative approach based on local Dirichlet forms is sketched at the end of the section.

Consider in $L^2(\mathbb{R}^3)$ the nonnegative operator

$$-\Delta|_{C_0^\infty(\mathbb{R}^3-\{y\})}, \qquad y \in \mathbb{R}^3, \tag{1.1.1}$$

where $\Delta = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$ is the Laplacian and denote by $\dot{H}_y$ its closure in $L^2(\mathbb{R}^3)$ (i.e., $\mathscr{D}(\dot{H}_y) = H_0^{2,2}(\mathbb{R}^3 - \{y\})$). By [274] (cf. also [276]) its adjoint can be characterized by

$$\dot{H}_y^* = -\Delta, \quad \mathscr{D}(\dot{H}_y^*) = \{g \in H_{\text{loc}}^{2,2}(\mathbb{R}^3 - \{y\}) \cap L^2(\mathbb{R}^3) | \Delta g \in L^2(\mathbb{R}^3)\}, \quad y \in \mathbb{R}^3, \tag{1.1.2}$$

where $H_{\text{loc}}^{m,n}(\Omega)$ denote the corresponding local Sobolev spaces (see, e.g., [389], Ch. IX). A straightforward computation shows that

$$\psi(k, x) = e^{ik|x-y|}/|x - y|, \qquad x \in \mathbb{R}^3 - \{y\}, \quad \text{Im } k > 0, \tag{1.1.3}$$

is the unique solution of

$$\dot{H}_y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \text{Im } k > 0. \tag{1.1.4}$$

Consequently, $\dot{H}_y$ has deficiency indices (1, 1) and applying Theorem A.1 all self-adjoint extensions $H_{\theta,y}$ of $\dot{H}_y$ are given by the one-parameter family

$$\begin{aligned} \mathscr{D}(H_{\theta,y}) &= \{g + c\psi_+ + ce^{i\theta}\psi_- \mid g \in \mathscr{D}(\dot{H}_y),\ c \in \mathbb{C}\}, \\ H_{\theta,y}(g + c\psi_+ + ce^{i\theta}\psi_-) &= \dot{H}_y g + ic\psi_+ - ice^{i\theta}\psi_-, \qquad \theta \in [0, 2\pi), \quad y \in \mathbb{R}^3, \end{aligned} \tag{1.1.5}$$

where

$$\psi_\pm(x) = e^{i\sqrt{\pm i}|x-y|}/(4\pi|x-y|), \qquad x \in \mathbb{R}^3 - \{y\}, \quad \operatorname{Im}\sqrt{\pm i} > 0. \tag{1.1.6}$$

Decomposing $L^2(\mathbb{R}^3)$ with respect to angular momenta, or, in other words, introducing spherical coordinates (with center y) we obtain (cf. [389], p. 160)

$$L^2(\mathbb{R}^3) = L^2((0, \infty); r^2\, dr) \otimes L^2(S^2), \tag{1.1.7}$$

where S^2 is the unit sphere in $\mathbb{R}^3$. The spherical harmonics $\{Y_{l,m} \mid l \in \mathbb{N}_0,\ m = 0, \pm 1, \ldots, \pm l\}$ provide a basis for $L^2(S^2)$. Using, in addition, the unitary transformation

$$U\colon L^2((0, \infty); r^2\, dr) \to L^2((0, \infty); dr), \qquad (Uf)(r) = rf(r), \tag{1.1.8}$$

we can write (1.1.7) as

$$L^2(\mathbb{R}^3) = \bigoplus_{l=0}^{\infty} U^{-1} L^2((0, \infty); dr) \otimes [Y_{l,-l}, \ldots, Y_{l,0}, \ldots, Y_{l,l}], \tag{1.1.9}$$

where $[f_1, \ldots, f_n]$ denotes the linear span of the vectors $f_1, \ldots, f_n$. With respect to this decomposition $\dot{H}_y$ equals the direct sum (cf. [389], p. 160)

$$\dot{H}_y = T_y^{-1} \left\{ \bigoplus_{l=0}^{\infty} U^{-1} \dot{h}_l U \otimes 1 \right\} T_y, \qquad y \in \mathbb{R}^3, \tag{1.1.10}$$

where T_y unitarily implements the translation $x \to x + y$ in $L^2(\mathbb{R}^3)$ (i.e., $(T_y g)(x) = g(x + y)$, $g \in L^2(\mathbb{R}^3)$, $y \in \mathbb{R}^3$) and

$$\begin{aligned} \dot{h}_l &= -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}, \qquad r > 0, \quad l = 0, 1, 2, \ldots, \\ \mathscr{D}(\dot{h}_0) &= \{\phi \in L^2((0, \infty)) \mid \phi, \phi' \in AC_{\text{loc}}((0, \infty));\ \phi(0+) = \phi'(0+) = 0; \\ &\qquad \phi'' \in L^2((0, \infty))\} = H_0^{2,2}((0, \infty)), \\ \mathscr{D}(\dot{h}_l) &= \{\phi \in L^2((0, \infty)) \mid \phi, \phi' \in AC_{\text{loc}}((0, \infty)); \\ &\qquad -\phi'' + l(l+1)r^{-2}\phi \in L^2((0, \infty))\}, \qquad l \geq 1. \end{aligned} \tag{1.1.11}$$

Here $AC_{\text{loc}}((a, b))$ denotes the set of locally absolutely continuous functions on (a, b).

By standard results (e.g., [389], Ch. X) $\dot{h}_l$, $l \geq 1$, are self-adjoint whereas $\dot{h}_0$ has deficiency indices (1, 1). In particular, all self-adjoint extensions $h_{0,\alpha}$ of $\dot{h}_0$

may be parametrized by (cf. Appendix D)

$$h_{0,\alpha} = -\frac{d^2}{dr^2},$$

$$\mathscr{D}(h_{0,\alpha}) = \{\phi \in L^2((0,\infty)) | \phi, \phi' \in AC_{\text{loc}}((0,\infty)); -4\pi\alpha\phi(0+) + \phi'(0+) = 0;$$
$$\phi'' \in L^2((0,\infty))\}, \qquad -\infty < \alpha \leq \infty. \tag{1.1.12}$$

(In obvious notation the boundary condition $\alpha = \infty$ denotes the Friedrichs extension characterized by $\phi(y+) = 0$.) From $\tilde{g}(r) = rg(r)$, $\tilde{g} \in \mathscr{D}(\dot{h}_0)$ and

$$\frac{d}{dr}[\tilde{g}(r) + c(4\pi)^{-1}e^{i\sqrt{i}r} + c(4\pi)^{-1}e^{i\theta}e^{i\sqrt{-i}r}]|_{r=0+}$$
$$= c(4\pi)^{-1}(e^{3\pi i/4} - e^{i\theta}e^{i\pi/4})$$
$$= 4\pi\alpha[\tilde{g}(r) + c(4\pi)^{-1}e^{i\sqrt{i}r} + c(4\pi)^{-1}e^{i\theta}e^{i\sqrt{-i}r}]|_{r=0+}, \tag{1.1.13}$$

where

$$\alpha = (4\pi)^{-1}\cos(\pi/4)[\tan(\theta/2) - 1], \tag{1.1.14}$$

we infer

$$H_{\theta,y} = T_y^{-1}\left\{\left[U^{-1}h_{0,\alpha}U \oplus \bigoplus_{l=1}^{\infty} U^{-1}\dot{h}_l U\right] \otimes 1\right\} T_y. \tag{1.1.15}$$

Obviously, α varies in $\mathbb{R}$ ($\alpha = +\infty$ if $\theta \uparrow \pi$) if θ varies in $[0, \pi) \cup (\pi, 2\pi)$. Thus we have proved

Theorem 1.1.1. *All self-adjoint extensions of $\dot{H}_y$ are given by*

$$-\Delta_{\alpha,y} = T_y^{-1}\left\{\left[U^{-1}h_{0,\alpha}U \oplus \bigoplus_{l=1}^{\infty} U^{-1}\dot{h}_l U\right] \otimes 1\right\} T_y,$$
$$-\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3. \tag{1.1.16}$$

The special case $\alpha = \infty$ just leads to the kinetic energy Hamiltonian $-\Delta$ (the Friedrichs extension of $\dot{H}_y$) in $L^2(\mathbb{R}^3)$

$$-\Delta_{\infty,y} = -\Delta \quad \textit{on} \quad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3). \tag{1.1.17}$$

If $|\alpha| < \infty$, $-\Delta_{\alpha,y}$ describes a *point interaction centered at* $y \in \mathbb{R}^3$. It will turn out in Sect. 1.4 that $-(4\pi\alpha)^{-1}$ represents the *scattering length* of $-\Delta_{\alpha,y}$. Denoting

$$G_k = (-\Delta - k^2)^{-1}, \qquad \operatorname{Im} k > 0 \tag{1.1.18}$$

it is well known (see, e.g., [389], p. 58f) that in three dimensions G_k has an integral kernel $G_k(x - x')$ given by

$$G_k(x - x') = e^{ik|x-x'|}/4\pi|x - x'|, \qquad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}^3, \quad x \neq x'. \tag{1.1.19}$$

In the following we characterize basic properties of $-\Delta_{\alpha,y}$. We start with

Theorem 1.1.2. *The resolvent of $-\Delta_{\alpha,y}$ is given by*

$$(-\Delta_{\alpha,y} - k^2)^{-1} = G_k + (\alpha - ik/4\pi)^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y),$$
$$k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3, \quad (1.1.20)$$

with integral kernel

$$(-\Delta_{\alpha,y} - k^2)^{-1}(x, x') = \frac{e^{ik|x-x'|}}{4\pi|x - x'|} + (\alpha - ik/4\pi)^{-1}\frac{e^{ik|x-y|}}{4\pi|x - y|}\frac{e^{ik|y-x'|}}{4\pi|y - x'|},$$
$$k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}^3, \quad x \neq x', \quad x \neq y, \quad x' \neq y. \quad (1.1.21)$$

PROOF. Using eq. (1.1.19), eq. (1.1.20) (except for the factor $(\alpha - ik/4\pi)^{-1}$) follows from (1.1.6) and Theorem A.2. To determine the missing factor it suffices to discuss eq. (1.1.20) in the subspace of angular momentum zero. Let $\eta \in L^2((0, \infty))$ and define

$$\chi_\alpha(r) = \int_0^\infty dr'\, g_0(k, r, r')\eta(r') + (4\pi\alpha - ik)^{-1}\int_0^\infty dr'\, e^{ikr'}\eta(r')e^{ikr},$$
$$\operatorname{Im} k > 0, \quad -\infty < \alpha \leq \infty, \quad (1.1.22)$$

where

$$g_0(k, r, r') = \begin{cases} k^{-1}\sin(kr)e^{ikr'}, & r \leq r', \\ k^{-1}\sin(kr')e^{ikr}, & r \geq r', \end{cases} \quad (1.1.23)$$

is the Green's function corresponding to $h_{0,\infty}$ (the Friedrichs extension of $\dot{h}_0$). Clearly, $\chi_\alpha, \chi'_\alpha \in AC_{\mathrm{loc}}((0, \infty))$ and $\chi_\alpha \in L^2((0, \infty))$. Moreover, a direct calculation shows that

$$-4\pi\alpha\chi_\alpha(0+) + \chi'_\alpha(0+) = 0 \quad (1.1.24)$$

and

$$\chi''_\alpha(r) = -\eta(r) - k^2\chi_\alpha(r), \quad r > 0, \quad (1.1.25)$$

which proves (1.1.20). ∎

Next we would like to collect some additional information on the domain of $-\Delta_{\alpha,y}$ and to show that the one-center point interaction is in fact a local interaction:

Theorem 1.1.3. *The domain $\mathscr{D}(-\Delta_{\alpha,y})$, $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}^3$, consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + (\alpha - ik/4\pi)^{-1}\phi_k(y)G_k(x - y), \quad x \neq y, \quad (1.1.26)$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3)$ and $k^2 \in \rho(-\Delta_{\alpha,y})$, $\operatorname{Im} k > 0$. The decomposition (1.1.26) is unique and with $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ of this form we obtain

$$(-\Delta_{\alpha,y} - k^2)\psi = (-\Delta - k^2)\phi_k. \quad (1.1.27)$$

Next, let $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ *and assume that* $\psi = 0$ *in an open set* $U \subseteq \mathbb{R}^3$. *Then* $-\Delta_{\alpha,y}\psi = 0$ *in* U.

Proof. We first note that functions in $H^{2,2}(\mathbb{R}^3)$ are Hölder continuous of exponent smaller than $\frac{1}{2}$ ([283], p. 301) and hence it makes sense to write $\phi_k(y)$. Next, we infer that

$$\begin{aligned}\mathscr{D}(-\Delta_{\alpha,y}) &= (-\Delta_{\alpha,y} - k^2)^{-1}(-\Delta - k^2)\mathscr{D}(-\Delta)\\ &= \{G_k + (\alpha - ik/4\pi)^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y)\}(-\Delta - k^2)\mathscr{D}(-\Delta),\\ &\qquad k^2 \in \rho(-\Delta_{\alpha,y}),\quad \operatorname{Im} k > 0, \end{aligned}\tag{1.1.28}$$

which proves (1.1.26). To prove uniqueness of the above decomposition let $\psi = 0$. Then

$$\phi_k(x) = -(\alpha - ik/4\pi)^{-1}\phi_k(y)G_k(x - y) \tag{1.1.29}$$

and $\phi_k \in C^0(\mathbb{R}^3)$, in fact, implies $\phi_k = 0$. Relation (1.1.27) then simply follows from

$$\begin{aligned}&(-\Delta_{\alpha,y} - k^2)^{-1}(-\Delta - k^2)\phi_k\\ &\quad = \phi_k + (\alpha - ik/4\pi)^{-1}(\overline{G_k(\cdot - y)}, (-\Delta - k^2)\phi_k)G_k(\cdot - y) = \psi,\\ &\qquad k^2 \in \rho(-\Delta_{\alpha,y}),\quad \operatorname{Im} k > 0. \end{aligned}\tag{1.1.30}$$

To prove locality (cf. also Lemma C.2) assume first $y \notin U$. Then

$$((-\Delta - k^2)G_k(\cdot - y))(x) = 0$$

implies that

$$\begin{aligned}(-\Delta_{\alpha,y}\psi)(x) &= k^2\psi(x) + ((-\Delta - k^2)\phi_k)(x)\\ &= -(\alpha - ik/4\pi)^{-1}\phi_k(y)((-\Delta - k^2)G_k(\cdot - y))(x) = 0, \qquad x \in U. \end{aligned}\tag{1.1.31}$$

On the other hand, if $y \in U$ then $\psi(y) = 0$ and $\phi_k \in C^0(\mathbb{R}^3)$ implies $\phi_k = 0$ and hence again

$$(-\Delta_{\alpha,y}\psi)(x) = k^2\psi(x) = 0, \qquad x \in U. \tag{1.1.32}$$

■

Finally, we turn to spectral properties of $-\Delta_{\alpha,y}$:

Theorem 1.1.4. *Let* $-\infty < \alpha \le \infty$, $y \in \mathbb{R}^3$. *Then the essential spectrum* $\sigma_{\text{ess}}(-\Delta_{\alpha,y})$ *is purely absolutely continuous and covers the nonnegative real axis*

$$\sigma_{\text{ess}}(-\Delta_{\alpha,y}) = \sigma_{\text{ac}}(-\Delta_{\alpha,y}) = [0, \infty), \qquad \sigma_{\text{sc}}(-\Delta_{\alpha,y}) = \varnothing. \tag{1.1.33}$$

(Here σ_{ac} *and* σ_{sc} *denote the absolutely and singularly continuous spectrum, respectively.) If* $\alpha < 0$, $-\Delta_{\alpha,y}$ *has precisely one negative, simple eigenvalue, i.e., its point spectrum* $\sigma_p(-\Delta_{\alpha,y})$ *is given by*

$$\sigma_p(-\Delta_{\alpha,y}) = \{-(4\pi\alpha)^2\}, \qquad -\infty < \alpha < 0, \tag{1.1.34}$$

with

$$4\pi(-\alpha)^{1/2}G_{-4\pi i\alpha}(x - y) = (-\alpha)^{1/2}e^{4\pi\alpha|x-y|}/|x - y|, \qquad x \neq y, \tag{1.1.35}$$

its strictly positive (normalized) eigenfunction. If $\alpha \geq 0$, $-\Delta_{\alpha,y}$ *has no eigenvalues, i.e.,*

$$\sigma_p(-\Delta_{\alpha,y}) = \varnothing, \qquad 0 \leq \alpha \leq \infty. \tag{1.1.36}$$

PROOF. Let $|\alpha| < \infty$. Weyl's theorem ([391], p. 112) and (1.1.20) imply $\sigma_{\text{ess}}(-\Delta_{\alpha,y}) = \sigma_{\text{ess}}(-\Delta) = [0, \infty)$ since $(-\Delta_{\alpha,y} - k^2)^{-1} - (-\Delta - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$, $-\infty < \alpha < \infty$, is of rank one. The absence of $\sigma_{\text{sc}}(-\Delta_{\alpha,y})$ follows, e.g., from Theorem XIII.20 of [391] together with (1.1.20). Assertion (1.1.34) and (1.1.35) and the absence of negative eigenvalues of $-\Delta_{\alpha,y}$ for $\alpha \geq 0$ then follow from the explicit structure of the residuum at $k = -4\pi i\alpha$ of (1.1.20). It remains to prove the absence of nonnegative eigenvalues for all $\alpha \in \mathbb{R}$. From the decomposition (1.1.16) we infer that it is sufficient to consider s-waves ($l = 0$). But this trivially follows from the fact that for $r > 0$ all solutions of

$$-\psi''(k, r) = k^2\psi(k, r), \qquad k \geq 0, \quad r > 0, \tag{1.1.37}$$

are given by

$$\begin{aligned} \psi(k, r) &= c_1 e^{ikr} + c_2 e^{-ikr}, \qquad k > 0, \\ \psi(0, r) &= c_3 + c_4 r, \qquad k = 0, \end{aligned} \tag{1.1.38}$$

which cannot be in $L^2((0, \infty))$. ∎

So far, we have discussed the approach based on operator extensions. Following [32], [33] we finally sketch another method using *local Dirichlet forms*. In $L^2(\mathbb{R}^3; \phi_\alpha^2\, d^3x)$ we define the energy form

$$\dot{E}_{\alpha,y}(g, h) = \int_{\mathbb{R}^3} \phi_{\alpha,y}^2(x)\, d^3x \overline{(\nabla g)(x)}(\nabla h)(x), \qquad \mathscr{D}(\dot{E}_{\alpha,y}) = C_0^1(\mathbb{R}^3), \qquad y \in \mathbb{R}^3, \tag{1.1.39}$$

where

$$\phi_{\alpha,y}(x) = \begin{cases} e^{4\pi\alpha|x-y|}/|x - y|, & \alpha \in \mathbb{R}, \quad x \in \mathbb{R}^3 - \{y\}, \\ 1, & \alpha = \infty. \end{cases} \tag{1.1.40}$$

It turns out that $\dot{E}_{\alpha,y}$ is closable and the unique self-adjoint operator associated with its closure is precisely the operator $\phi_{\alpha,y}^{-1}[-\Delta_{\alpha,y} + (4\pi\alpha)^2]\phi_{\alpha,y}$ if $\alpha \in \mathbb{R}$ (resp. $-\Delta$ if $\alpha = \infty$) (cf. Appendix F). For a construction of $(-\Delta_{\alpha,y} - k^2)^{-1}$ by means of *nonstandard analysis* we refer to [12], [14] and Appendix H.

Obviously, the results of this section are not confined to self-adjoint extensions (i.e., $\alpha \in \mathbb{R}$) of $\dot{H}_y$ but straightforwardly extend to accretive extensions ([389], Ch. X) of $i\dot{H}_y$ if $\operatorname{Im} \alpha < 0$. In this way, complex point interactions are obtained (cf. Theorem 2.1.4).

Since $-\Delta|_{C_0^\infty(\mathbb{R}^n - \{y\})}$, $y \in \mathbb{R}^n$, $n \in \mathbb{N}$, is essentially self-adjoint in $L^2(\mathbb{R}^n)$ if $n \geq 4$ ([389], Ch. X), there are no point interactions in more than three dimensions. On the other hand, operators of the type

$$(-\Delta + \lambda|\cdot - y|^{-2})|_{C_0^\infty(\mathbb{R}^n - \{y\})}, \qquad -[(n-2)/2]^2 < \lambda < 1 - [(n-2)/2]^2, \tag{1.1.41}$$

certainly admit self-adjoint extensions which correspond to an interaction given by $\lambda|x - y|^{-2}$ plus point interaction centered at y as discussed in [209].

I.1.2 Approximations by Means of Local as well as Nonlocal Scaled Short-Range Interactions

The question as to under what circumstances $-\Delta_{\alpha,y}$ can be obtained as a norm resolvent limit of scaled short-range Hamiltonians is answered in this section. We first treat the case of local interactions. Recall that

$$G_k = (-\Delta - k^2)^{-1}, \qquad \text{Im } k > 0, \tag{1.2.1}$$

denotes the "free" resolvent with integral kernel

$$G_k(x - x') = e^{ik|x-x'|}/4\pi|x - x'|, \qquad \text{Im } k > 0, \quad x, x' \in \mathbb{R}^3, \quad x \neq x', \tag{1.2.2}$$

and assume $V: \mathbb{R}^3 \to \mathbb{R}$ to be measurable and belonging to the *Rollnik class R*, i.e., $\|V\|_R^2 \equiv \int_{\mathbb{R}^6} d^3x\, d^3x' |V(x)||V(x')||x - x'|^{-2} < \infty$. For the general theory of Rollnik functions, see [434]. We also introduce

$$v(x) = |V(x)|^{1/2}, \qquad u(x) = |V(x)|^{1/2} \operatorname{sgn}[V(x)] \tag{1.2.3}$$

and note

Lemma 1.2.1. *Let $V \in R$. Then V is form compact with respect to $-\Delta$, i.e.,*

$$|V|^{1/2}(-\Delta + E)^{-1/2} \in \mathscr{B}_\infty(L^2(\mathbb{R}^3)), \qquad E > 0, \tag{1.2.4}$$

and

$$uG_kv \in \mathscr{B}_2(L^2(\mathbb{R}^3)), \qquad \text{Im } k \geq 0. \tag{1.2.5}$$

PROOF. Equation (1.2.4) follows from (1.2.5) which in turn is a direct consequence of $V \in R$ and dominated convergence. ∎

In addition, we define

$$\tilde{v}(x) = v(x - \varepsilon^{-1}y), \qquad \tilde{u}(x) = u(x - \varepsilon^{-1}y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3, \tag{1.2.6}$$

and

$$\tilde{B}(\varepsilon, k) = \lambda(\varepsilon)\tilde{u}G_k\tilde{v}, \qquad \text{Im } k > 0, \quad \varepsilon > 0, \tag{1.2.7}$$

where $\lambda(\cdot)$ is real-analytic near the origin with $\lambda(0) = 1$. Because of (1.2.5), $\tilde{B}(\varepsilon, k)$ extends to a Hilbert–Schmidt operator for $\text{Im } k \geq 0$. Moreover, by eq. (1.2.4) and by Appendix B, the form sum

$$H_y(\varepsilon) = -\Delta \dotplus \lambda(\varepsilon)V(\cdot - \varepsilon^{-1}y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3, \tag{1.2.8}$$

is well defined and by Theorem B.1(b) the resolvent equation

$$(H_y(\varepsilon) - k^2)^{-1} = G_k - \lambda(\varepsilon)G_k\tilde{v}[1 + \tilde{B}(\varepsilon, k)]^{-1}\tilde{u}G_k,$$
$$k^2 \in \rho(H_y(\varepsilon)), \quad \text{Im } k > 0, \quad y \in \mathbb{R}^3, \tag{1.2.9}$$

holds. To obtain suitable scaled short-range Hamiltonians $H_{\varepsilon,y}$ we denote by U_ε the unitary scaling group

$$(U_\varepsilon g)(x) = \varepsilon^{-3/2}g(x/\varepsilon), \qquad \varepsilon > 0, \quad g \in L^2(\mathbb{R}^3), \tag{1.2.10}$$

and define

$$\begin{aligned} H_{\varepsilon,y} &= \varepsilon^{-2}U_\varepsilon H_y(\varepsilon)U_\varepsilon^{-1} = -\Delta \dotplus V_{\varepsilon,y}, \\ V_{\varepsilon,y}(x) &= \lambda(\varepsilon)\varepsilon^{-2}V((x-y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3. \end{aligned} \tag{1.2.11}$$

In order to discuss the limit $\varepsilon \downarrow 0$ of $H_{\varepsilon,y}$ we first introduce Hilbert–Schmidt operators $A_\varepsilon(k)$, $B_\varepsilon(k) = \lambda(\varepsilon)uG_{\varepsilon k}v$, $C_\varepsilon(k)$, $\varepsilon > 0$, with integral kernels

$$A_\varepsilon(k, x, x') = G_k(x - y - \varepsilon x')v(x'), \qquad \operatorname{Im} k > 0, \tag{1.2.12}$$

$$B_\varepsilon(k, x, x') = \lambda(\varepsilon)u(x)G_{\varepsilon k}(x - x')v(x'), \qquad \operatorname{Im} k \geq 0, \tag{1.2.13}$$

$$C_\varepsilon(k, x, x') = u(x)G_k(\varepsilon x + y - x'), \qquad \operatorname{Im} k > 0. \tag{1.2.14}$$

Then, using

$$\varepsilon^2 U_\varepsilon G_k U_\varepsilon^{-1} = G_{k/\varepsilon}, \qquad \varepsilon > 0, \tag{1.2.15}$$

we infer from (1.2.9) using translations $x \to x + (y/\varepsilon)$, $\varepsilon > 0$,

$$\begin{aligned} (H_{\varepsilon,y} - k^2)^{-1} &= \varepsilon^2 U_\varepsilon[H_y(\varepsilon) - (\varepsilon k)^2]^{-1}U_\varepsilon^{-1} \\ &= G_k - \lambda(\varepsilon)A_\varepsilon(k)\varepsilon[1 + B_\varepsilon(k)]^{-1}C_\varepsilon(k), \\ &\qquad k^2 \in \rho(H_{\varepsilon,y}), \quad \operatorname{Im} k > 0. \end{aligned} \tag{1.2.16}$$

Lemma 1.2.2. *Let $y \in \mathbb{R}^3$ and define rank-one operators $A(k)$, $C(k)$, and the Hilbert–Schmidt operator uG_0v with kernels*

$$A(k, x, x') = G_k(x - y)v(x'), \qquad \operatorname{Im} k > 0, \quad x \neq y, \tag{1.2.17}$$

$$(uG_0v)(x, x') = u(x)(4\pi|x - x'|)^{-1}v(x'), \qquad x \neq x', \tag{1.2.18}$$

$$C(k, x, x') = u(x)G_k(y - x'), \qquad \operatorname{Im} k > 0, \quad x' \neq y. \tag{1.2.19}$$

Then for fixed k, $\operatorname{Im} k > 0$, $A_\varepsilon(k)$, $B_\varepsilon(k)$, $C_\varepsilon(k)$ converge in Hilbert–Schmidt norm to $A(k)$, uG_0v, $C(k)$, respectively, as $\varepsilon \downarrow 0$.

PROOF. By dominated convergence

$$\operatorname*{w-lim}_{\varepsilon\downarrow 0} A_\varepsilon(k) = A(k), \qquad \operatorname*{w-lim}_{\varepsilon\downarrow 0} B_\varepsilon(k) = uG_0v, \qquad \operatorname*{w-lim}_{\varepsilon\downarrow 0} C_\varepsilon(k) = C(k). \tag{1.2.20}$$

Since, obviously,

$$\lim_{\varepsilon\downarrow 0} \|A_\varepsilon(k)\|_2 = \|A(k)\|_2, \qquad \lim_{\varepsilon\downarrow 0} \|B_\varepsilon(k)\|_2 = \|uG_0v\|_2, \qquad \lim_{\varepsilon\downarrow 0} \|C_\varepsilon(k)\|_2 = \|C(k)\|_2, \tag{1.2.21}$$

the assertion follows by Theorem 2.21 of [438]. ∎

So far the whole analysis did not use any particular spectral informations about the underlying Hamiltonians. However, in order to determine the limit $\varepsilon \downarrow 0$ of $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ we have to take into account zero-energy spectral properties of

$$\tilde{H}_y(\varepsilon) = -\Delta \dotplus V(\cdot - \varepsilon^{-1}y) \tag{1.2.22}$$

or by unitary equivalence (translations) zero-energy properties of

$$H = -\Delta \dotplus V. \tag{1.2.23}$$

Therefore we introduce below, after Lemma 1.2.3, the notion of a zero-energy resonance (resp. a zero-energy bound state) of H. Assume now, in addition, $V \in L^1(\mathbb{R}^3)$. If

$$uG_0 v\phi = -\phi \qquad \text{for some} \quad \phi \in L^2(\mathbb{R}^3) \tag{1.2.24}$$

we define

$$\psi(x) = (G_0 v\phi)(x). \tag{1.2.25}$$

Lemma 1.2.3. *Suppose $V \in L^1(\mathbb{R}^3) \cap R$. Then $\psi \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$, $\nabla\psi \in L^2(\mathbb{R}^3)$, and $H\psi = 0$ in the sense of distributions. If, in addition, $|\cdot|\, V \in L^1(\mathbb{R}^3)$, then $\psi \in L^2(\mathbb{R}^3)$ is equivalent to*

$$(v, \phi) = -\int_{\mathbb{R}^3} d^3x\; V(x)\psi(x) = 0. \tag{1.2.26}$$

If $\psi \in L^2(\mathbb{R}^3)$, then $\psi \in \mathscr{D}(H)$ and $H\psi = 0$.

PROOF. From

$$\psi(x) = (4\pi|x|)^{-1}(v, \phi) + \psi_1(x), \tag{1.2.27}$$

where

$$\psi_1(x) = (4\pi)^{-1} \int_{\mathbb{R}^3} d^3x'(|x - x'|^{-1} - |x|^{-1})v(x')\phi(x'), \tag{1.2.28}$$

and the fact that

$$\int_{|x| \le r} d^3x(|x - x'|^{-1} - |x|^{-1})^2 \le cr \tag{1.2.29}$$

and

$$\int_{\mathbb{R}^3} d^3x(|x - x'|^{-1} - |x|^{-1})^2 \le \tilde{c}|x'| \tag{1.2.30}$$

for appropriate constants $c, \tilde{c} > 0$, one infers that $\psi_1 \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$ if $V \in L^1(\mathbb{R}^3)$, and $\psi_1 \in L^2(\mathbb{R}^3)$ if $|\cdot|\, V \in L^1(\mathbb{R}^3)$. Moreover,

$$(\nabla\psi)(x) = -\int d^3x'(4\pi)^{-1}|x - x'|^{-3}(x - x')v(x')\phi(x'), \tag{1.2.31}$$

in the sense of distributions, and Fubini's theorem imply

$$\begin{aligned}
&\int_{\mathbb{R}^3} d^3x|(\nabla\psi)(x)|^2 \\
&\le (4\pi)^{-2} \int_{\mathbb{R}^6} d^3x'\, d^3x''\, v(x')v(x'')|\phi(x')||\phi(x'')| \int_{\mathbb{R}^3} d^3x|x - x'|^{-2}|x - x''|^{-2} \\
&= d(4\pi)^{-2} \int_{\mathbb{R}^6} d^3x'\, d^3x''|x' - x''|^{-1}v(x')v(x'')|\phi(x')||\phi(x'')| \\
&\le d(4\pi)^{-2}\|V\|_R\|\phi\|^2 < \infty,
\end{aligned} \tag{1.2.32}$$

where

$$d = \int_{\mathbb{R}^3} d^3z |z|^{-2} |z - e_3|^{-2} < \infty$$

(e_3 the unit vector in the z_3-direction). Since $v\psi = -(\operatorname{sgn} V)\phi \in L^2(\mathbb{R}^3)$, $\nabla\psi$ defines a distribution (cf. Corollary II.8(a) in [434]) and $-\Delta\psi + V\psi = 0$ in the sense of distributions. If $\psi \in L^2(\mathbb{R}^3)$ then $\psi \in \mathscr{D}(H)$ by Corollary II. 8(a)) of [434]. ∎

If $\psi \in L^2(\mathbb{R}^3)$, then ψ is a *zero-energy eigenstate* of H and $0 \in \sigma_p(H)$. If $\psi \in L^2_{\text{loc}}(\mathbb{R}^3)$, but $\psi \notin L^2(\mathbb{R}^3)$ we call ψ a *zero-energy resonance function* of H and the spectral point 0 a *resonance* of H. Lemma 1.2.3 is a convenient tool to decide whether 0 is a zero-energy bound state (resp. resonance) of H. We thus distinguish the following cases:

Case I: -1 is not an eigenvalue of uG_0v.

Case II: -1 is a simple eigenvalue of uG_0v,

$$uG_0v\phi = -\phi, \qquad \phi \in L^2(\mathbb{R}^3)$$

and

$$\psi = G_0v\phi \in L^2_{\text{loc}}(\mathbb{R}^3),$$

but $\psi \notin L^2(\mathbb{R}^3)$.

Case III: -1 is an eigenvalue of uG_0v,

$$uG_0v\phi_l = -\phi_l, \qquad \phi_l \in L^2(\mathbb{R}^3), \quad l = 1, \ldots, N,$$

and

$$\psi_l = G_0v\phi_l \in L^2(\mathbb{R}^3), \qquad l = 1, \ldots, N.$$

Case IV: -1 is an eigenvalue of uG_0v,

$$uG_0v\phi_l = -\phi_l, \qquad \phi_l \in L^2(\mathbb{R}^3), \quad l = 1, \ldots, N, \quad N \geq 2,$$
$$\psi_l = G_0v\phi_l \in L^2_{\text{loc}}(\mathbb{R}^3), \qquad l = 1, \ldots, N,$$

and at least one $\psi_{l_0} \notin L^2(\mathbb{R}^3)$.

Observe that the functions ϕ_l, ψ_l can be chosen to be real-valued. Clearly, case I is the generic one in the sense that if V is replaced by gV, $g \geq 0$, then cases II–IV only occur for discrete values of the coupling constant g. In particular, if $V \geq 0$ then only case I occurs. In case II, H has a simple zero-energy resonance; in case III, H has a zero-energy eigenvalue of multiplicity N. Since in case IV one can always choose a particular linear combination of the ϕ_l's such that $(v, \phi_1) \neq 0$ but $(v, \phi_l) = 0, l = 2, \ldots, N, H$ has a simple zero-energy resonance and a zero-energy eigenvalue of multiplicity $N - 1$ in case IV if $V \in R$ and $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$. If, in addition, V is spherically symmetric then $(v, \phi) = 0$ for all functions ϕ belonging to angular momentum $l \geq 1$. Thus case II (i.e. a zero-energy resonance) only occurs in s-waves whereas p- and higher waves only support zero-energy bound states. From now on we always assume $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$ in cases II–IV.

Given the above case distinction we can formulate

Lemma 1.2.4. *Let* $V \in R$. *In cases* II–IV *assume, in addition,* $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$ *and* $\lambda'(0) \neq 0$ *in cases* III *and* IV. *Then*

$$\underset{\varepsilon \downarrow 0}{\text{n-lim}}\, \varepsilon[1 + B_\varepsilon(k)]^{-1} = \begin{cases} 0 & \text{in case I,} \\ [(4\pi)^{-1} ik|(v, \phi)|^2 + \lambda'(0)]^{-1}(\tilde{\phi}, \cdot)\phi & \text{in case II,} \\ [\lambda'(0)]^{-1} \sum_{l=1}^{N} (\tilde{\phi}_l, \cdot)\phi_l & \text{in case III,} \\ \sum_{l,l'=1}^{N} (\tilde{\phi}, B_1(k)\phi)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l & \text{in case IV,} \end{cases} \tag{1.2.33}$$

where $k^2 \in \mathbb{C} - \mathbb{R}$, $\operatorname{Im} k > 0$, *and* $(\tilde{\phi}, B_1(k)\phi)_{ll'}^{-1}$ *denotes the inverse of the matrix* $(\tilde{\phi}_l, B_1(k)\phi_{l'})$

$$\begin{aligned} &\tilde{\phi}_l(x) = \operatorname{sgn}[V(x)]\phi_l(x), \qquad (\tilde{\phi}_l, \phi_{l'}) = -\delta_{ll'}, \qquad l, l' = 1, \ldots, N, \\ &B_1(k) = \lambda'(0)uG_0v + (4\pi)^{-1} ik(v, \cdot)u. \end{aligned} \tag{1.2.34}$$

Proof. *Case* I: Since $\text{n-lim}_{\varepsilon \downarrow 0} B_\varepsilon(k) = uG_0v$ and $(1 + uG_0v)^{-1}$ exists the result immediately follows.

In cases II–IV we first note the norm convergent expansion

$$(1 + uG_0v + z)^{-1} = z^{-1}P + \sum_{m=0}^{\infty} (-z)^m T^{m+1}, \qquad z \in \mathbb{C} - \{0\} \text{ small enough,} \tag{1.2.35}$$

where

$$P = -\sum_{l=1}^{N} (\tilde{\phi}_l, \cdot)\phi_l, \qquad \tilde{\phi}_l = (\operatorname{sgn} V)\phi_l, \quad l = 1, \ldots, N, \tag{1.2.36}$$

is the projection onto the eigenspace of uG_0v to the eigenvalue -1 and

$$T = \underset{z \to 0}{\text{n-lim}}\, (1 + z + uG_0v)^{-1}(1 - P) \tag{1.2.37}$$

denotes the corresponding reduced resolvent. Moreover, the ϕ_l can be chosen in such a way that

$$(\tilde{\phi}_l, \phi_{l'}) = -\delta_{ll'}, \qquad l, l' = 1, \ldots, N. \tag{1.2.38}$$

In order to prove (1.2.35)–(1.2.38) we first show that the algebraic and geometric multiplicity of the eigenvalue -1 of uG_0v coincide. For this purpose it suffices to prove that $(1 + uG_0v)^2 g = 0, g \in L^2(\mathbb{R}^3)$ implies $(1 + uG_0v)g = 0$: Assume $(1 + uG_0v)^2 g = 0$ and define $f = (1 + uG_0v)g$. Then $(1 + uG_0v)f = 0$ and, consequently,

$$(\tilde{f}, f) = ((1 + vG_0u)\tilde{g}, (1 + uG_0v)g) = (\tilde{g}, (1 + uG_0v)^2 g) = 0, \tag{1.2.39}$$

where

$$\tilde{f} = (1 + vG_0u)\tilde{g}, \qquad \tilde{g} = (\operatorname{sgn} V)g. \tag{1.2.40}$$

But $0 = -(\tilde{f}, uG_0vf) = -(G_0^{1/2}u\tilde{f}, G_0^{1/2}vf) = -\|G_0^{1/2}vf\|^2$ implies $vf = 0$ and hence

$f = 0$ (since $f = -uG_0vf$). By [283], Ch. III.6.5 we get an expansion of the type (1.2.35). It remains to show that the normalization (1.2.38) is indeed possible. This actually follows from

$$(\tilde{\phi}, \phi) = -(\tilde{\phi}, uG_0v\phi) = -\|G_0^{1/2}v\phi\|^2 \neq 0,$$
$$uG_0v\phi = -\phi, \qquad \phi \in L^2(\mathbb{R}^3), \qquad \tilde{\phi} = (\operatorname{sgn} V)\phi, \tag{1.2.41}$$

and the analog of the Gram–Schmidt orthogonalization process.

Next we remark that, due to the hypothesis $V \in R \cap L^1(\mathbb{R}^3)$, the expansion

$$B_\varepsilon(k) = uG_0v + \varepsilon\lambda'(0)uG_0v + \varepsilon(4\pi)^{-1}ik(v, \cdot)u + o(\varepsilon)$$
$$\equiv B_0 + \varepsilon B_1(k) + o(\varepsilon) \tag{1.2.42}$$

is valid in Hilbert–Schmidt norm for fixed k with $\operatorname{Im} k \geq 0$. Equation (1.2.42) is shown as follows: By the mean-value theorem

$$\lambda(\varepsilon)G_{\varepsilon k}(x, x') = G_0(x, x') - \varepsilon\lambda'(\varepsilon\tilde{\theta}(\varepsilon))G_0(x, x') + \varepsilon(4\pi)^{-1}ike^{i\varepsilon\theta(\varepsilon)k|x-x'|}, \qquad x \neq x', \tag{1.2.43}$$

for appropriate functions $0 \leq \theta(\varepsilon), \tilde{\theta}(\varepsilon) \leq 1$. Thus

$$\|B_\varepsilon(k) - uG_0v - \varepsilon\lambda'(0)uG_0v - \varepsilon(4\pi)^{-1}ik(v, \cdot)u\|_2^2$$
$$\leq 2\varepsilon^2|\lambda'(\varepsilon\tilde{\theta}(\varepsilon)) - \lambda'(0)|^2\|uG_0v\|_2^2$$
$$+ 2\varepsilon^2(4\pi)^{-2}|k|^2\int_{\mathbb{R}^6} d^3x\, d^3x'|V(x)||V(x')||e^{i\varepsilon\theta(\varepsilon)k|x-x'|} - 1|^2 = o(\varepsilon^2) \tag{1.2.44}$$

by dominated convergence. (A slightly more detailed estimate actually shows that $o(\varepsilon)$ can be replaced by $o(\varepsilon^{3/2})$ in (1.2.42) since $|\cdot|V \in L^1(\mathbb{R}^3)$.)

Case II: By eqs. (1.2.35) and (1.2.42)

$$\varepsilon[1 + B_\varepsilon(k)]^{-1}$$
$$= \varepsilon[1 + B_0 + \varepsilon B_1 + o(\varepsilon)]^{-1}$$
$$= [1 + \varepsilon(1 + \varepsilon + B_0)^{-1}(B_1 - 1 + o(\varepsilon))]^{-1}\varepsilon(1 + \varepsilon + B_0)^{-1}$$
$$= [1 + P(B_1 - 1) + o(\varepsilon)]^{-1}[P + O(\varepsilon)], \qquad k^2 \in \rho(H_{\varepsilon,y}), \quad \operatorname{Im} k > 0. \tag{1.2.45}$$

Since $[1 + P(B_1 - 1)]^{-1}$ is easily seen to exist as a bounded operator in $L^2(\mathbb{R}^3)$

$$[1 + P(B_1 - 1)]^{-1} = 1 + [(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}[1 + \lambda'(0)](\tilde{\phi}, \cdot)\phi$$
$$- (ik/4\pi)[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}(\phi, v)(v, \cdot)\phi \tag{1.2.46}$$

and from

$$[1 + P(B_1 - 1)]^{-1}P = [(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}(\tilde{\phi}, \cdot)\phi \tag{1.2.47}$$

we get (1.2.33).

Case III: Observing again that $[1 + P(B_1 - 1)]^{-1}$ exists,

$$[1 + P(B_1 - 1)]^{-1} = 1 + [1 + \lambda'(0)^{-1}]P, \tag{1.2.48}$$

and that

$$[1 + P(B_1 - 1)]^{-1}P = -[\lambda'(0)]^{-1}P, \tag{1.2.49}$$

in case III we obtain the desired result directly from (1.2.45).

Case IV: Here again $[1 + P(B_1 - 1)]^{-1}$ is a bounded operator

$$[1 + P(B_1 - 1)]^{-1} = 1 - \sum_{l,l'=1}^{N} (\tilde{\phi}, B_1\phi)^{-1}_{ll'}([B_1^* - 1]\tilde{\phi}_{l'}, \cdot)\phi_l \tag{1.2.50}$$

and inserting

$$[1 + P(B_1 - 1)]^{-1}P = \sum_{l,l'=1}^{N} (\tilde{\phi}, B_1\phi)^{-1}_{ll'}(\tilde{\phi}_{l'}, \cdot)\phi_l \tag{1.2.51}$$

into (1.2.45) completes the proof. (By inspection

$$\det[(\tilde{\phi}_l, B_1(k)\phi_{l'})] = [4\pi\lambda'(0)/ik]^{N-1}\left[\lambda'(0) + (4\pi)^{-1}ik \sum_{l=1}^{N} |(v, \phi_l)|^2\right].\Big) \qquad \blacksquare$$

From now on we always assume the normalization $(\tilde{\phi}, \phi) = -1$ in case II and $(\tilde{\phi}_l, \phi_{l'}) = -\delta_{ll'}$, $l, l' = 1, \ldots, N$, in cases III and IV.

Lemmas 1.2.2 and 1.2.4 now enable us to present the main result of this section.

Theorem 1.2.5. *Let $V \in R$ be real-valued and $y \in \mathbb{R}^3$. In cases* II–IV *assume, in addition, $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$ and $\lambda'(0) \neq 0$ in cases* III *and* IV. *Then, if $k^2 \in \rho(-\Delta_{\alpha,y})$, we get $k^2 \in \rho(H_{\varepsilon,y})$ for $\varepsilon > 0$ small enough and that $H_{\varepsilon,y}$ converges to $-\Delta_{\alpha,y}$ in norm resolvent sense as $\varepsilon \downarrow 0$, viz.*

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}, \qquad y \in \mathbb{R}^3, \tag{1.2.52}$$

where α is given by

$$\alpha = \begin{cases} \infty & \textit{in case I}, \\ -\lambda'(0)|(v, \phi)|^{-2} & \textit{in case II}, \\ \infty & \textit{in case III}, \\ -\lambda'(0)\left\{\sum_{l=1}^{N} |(v, \phi_l)|^2\right\}^{-1} & \textit{in case IV}. \end{cases} \tag{1.2.53}$$

In particular, $H_{\varepsilon,y}$ converges in norm resolvent sense to $-\Delta$ in cases I *and* III *as $\varepsilon \downarrow 0$.*

PROOF. Denoting the right-hand side of (1.2.33) by $D(k)$ we obtain from the resolvent equation (1.2.16), and from Lemmas 1.2.2 and 1.2.4 that

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} = G_k - A(k)D(k)C(k), \qquad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0. \tag{1.2.54}$$

Inserting the explicit result (1.2.33) into (1.2.54), using the criterion (1.2.26) yields (1.2.52) and (1.2.53) after comparison with (1.1.20). $\blacksquare$

As a consequence, if $\alpha < 0$ (i.e., $\lambda'(0) > 0$ in case II or IV), there exists a sequence of eigenvalues E_ε of $H_{\varepsilon,y}$ that converges to $-(4\pi\alpha)^2$ as $\varepsilon \downarrow 0$. Moreover, Theorem 1.2.5 implies strong convergence of the unitary (resp. semi-) groups associated with $H_{\varepsilon,y}$ to that of $-\Delta_{\alpha,y}$. Obviously, self-adjointness of $H_{\varepsilon,y}$ or $-\Delta_{\alpha,y}$ was inessential in the above proof and thus one also obtains strong convergence of the corresponding contraction semigroups $e^{-itH_{\varepsilon,y}}$,

$t \geq 0$, if, e.g., $V \leq 0$ ($V \geq 0$) and Im $\lambda \geq 0$ (Im $\lambda \leq 0$) to $e^{it\Delta_{\alpha,y}}$, $t \geq 0$, as $\varepsilon \downarrow 0$ ([389], Ch. X; [283], Ch. IX).

A look at (1.2.52) and (1.2.53) shows that, in general (i.e., in case I) $H_{\varepsilon,y}$ converges to $-\Delta$ as $\varepsilon \downarrow 0$. To illustrate this phenomenon we take, e.g.,

$$V(x) = (1 + |x|)^{-5}. \tag{1.2.55}$$

Then

$$V_{\varepsilon,y}(x) = \lambda(\varepsilon)\varepsilon^3(\varepsilon + |x - y|)^{-5}, \qquad y \in \mathbb{R}^3, \tag{1.2.56}$$

such that

$$\begin{aligned} H_{\varepsilon,y} &= -\Delta + [1 + \varepsilon\lambda'(0) + O(\varepsilon^2)]\varepsilon^3(\varepsilon + |x - y|)^{-5}, \\ \mathscr{D}(H_{\varepsilon,y}) &= \mathscr{D}(-\Delta), \qquad \varepsilon > 0. \end{aligned} \tag{1.2.57}$$

Thus for $x \neq y$

$$V_\varepsilon(x) \xrightarrow[\varepsilon\downarrow 0]{} 0 \quad \text{pointwise}, \tag{1.2.58}$$

which indicates that in the limit $\varepsilon \downarrow 0$ the resulting "potential" in $\lim_{\varepsilon\downarrow 0} H_{\varepsilon,y}$ should either vanish (like it does in cases I and III) or should be concentrated at $x = y$ (as in cases II and IV). It will become clear later on in Sect. 1.4 why only a zero-energy resonance of H forces $H_{\varepsilon,y}$ to converge to a point interaction Hamiltonian (centered at y) in the limit $\varepsilon \downarrow 0$. Since $H_{\varepsilon,y} = \varepsilon^{-2}U_\varepsilon H_y(\varepsilon)U_\varepsilon^{-1}$ and, moreover, $\tilde{H}_y(\varepsilon) = -\Delta \dotplus V(\cdot - \varepsilon^{-1}y)$ is unitarily equivalent (by translations) to $H = -\Delta \dotplus V$ it is intuitively clear that the limit of $H_{\varepsilon,y}$ as $\varepsilon \downarrow 0$ depends on the asymptotic behavior of $H_{\varepsilon,y}$ in configuration space or equivalently, on the low-energy behavior of $\tilde{H}_y(\varepsilon)$ and hence of H.

Now we turn to the discussion of *nonlocal interactions*. Let W be a self-adjoint trace class operator in $L^2(\mathbb{R}^3)$, $W \in \mathscr{B}_1(L^2(\mathbb{R}^3))$. In addition, assume that W can be written as the product of two Hilbert–Schmidt operators $W_1, W_2 \in \mathscr{B}_2(L^2(\mathbb{R}^3))$

$$W = W_1 W_2 \tag{1.2.59}$$

such that the integral kernels $W_j(x, x')$ of W_j, $j = 1, 2$, satisfy

$$\tilde{\tilde{u}}_1, \tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3), \tag{1.2.60}$$

where

$$\tilde{\tilde{u}}_1(x) = \left(\int_{\mathbb{R}^3} d^3x' \, |W_1(x, x')|^2\right)^{1/2}, \qquad \tilde{\tilde{v}}_2(x') = \left(\int_{\mathbb{R}^3} d^3x \, |W_2(x, x')|^2\right)^{1/2}. \tag{1.2.61}$$

Then the analog of Lemma 1.2.1 reads

Lemma 1.2.6. *Let W_j, $j = 1, 2$, be as above. Then W is relatively compact with respect to $-\Delta$ and*

$$W_2 G_k W_1 \in \mathscr{B}_2(L^2(\mathbb{R}^3)), \qquad \text{Im } k \geq 0. \tag{1.2.62}$$

PROOF. Since $W \in \mathscr{B}_1(L^2(\mathbb{R}^3))$, it is obviously relatively compact with respect to $-\Delta$. In order to prove (1.2.62) we observe that

$$\begin{aligned}\|W_2 G_k W_1\|_2^2 &= \int_{\mathbb{R}^{18}} d^3z\, d^3z'\, d^3x\, d^3x'\, d^3y\, d^3y'\, W_2(z,x) \frac{e^{ik|x-y|}}{4\pi|x-y|} W_1(y,z') \cdot \\ &\quad \cdot \overline{W_2(z',x')} \frac{e^{-i\bar{k}|x'-y'|}}{4\pi|x'-y'|} \overline{W_1(y',z')} \\ &\le \int_{\mathbb{R}^{12}} d^3x\, d^3y\, d^3x'\, d^3y' \frac{\tilde{\tilde{v}}_2(x)\tilde{\tilde{u}}_1(y)}{4\pi|x-y|} \frac{\tilde{\tilde{v}}_2(x')\tilde{\tilde{u}}_1(y')}{4\pi|x'-y'|} \\ &= \left(\int_{\mathbb{R}^6} d^3x\, d^3y \frac{\tilde{\tilde{v}}_2(x)\tilde{\tilde{u}}_1(y)}{4\pi|x-y|}\right)^2 \le C\|\tilde{\tilde{v}}_2\|_{6/5}^2 \|\tilde{\tilde{u}}_1\|_{6/5}^2, \qquad \operatorname{Im} k \ge 0,\end{aligned} \tag{1.2.63}$$

by Sobolev's inequality (cf. Lemma B.6). ■

The analog of the operator (1.2.23) (we again call it H) is then given by

$$H = -\Delta + W \quad \text{on} \quad \mathscr{D}(H) = H^{2,2}(\mathbb{R}^3) \tag{1.2.64}$$

and the scaled short-range Hamiltonian $H_{\varepsilon,y}$ now reads

$$\begin{aligned}H_{\varepsilon,y} &= \varepsilon^{-2} U_\varepsilon T_{y/\varepsilon}^{-1} [-\Delta + \lambda(\varepsilon) W] T_{y/\varepsilon} U_\varepsilon^{-1} = -\Delta + W_{\varepsilon,y}, \\ W_{\varepsilon,y}(x,x') &= \varepsilon^{-5}\lambda(\varepsilon) W(\varepsilon^{-1}(x-y), \varepsilon^{-1}(x'-y)), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3,\end{aligned} \tag{1.2.65}$$

where $\lambda(\cdot)$ has been introduced in (1.2.7), U_ε denotes the unitary scaling group (1.2.10), and T_y unitarily implements translations $x \to x + y$ in $L^2(\mathbb{R}^3)$ (cf. (1.1.10)). Similar to (1.2.16), one obtains

$$\begin{aligned}(H_{\varepsilon,y} - k^2)^{-1} &= G_k - \lambda(\varepsilon) A_\varepsilon(k) \varepsilon [1 + B_\varepsilon(k)]^{-1} C_\varepsilon(k), \\ &\qquad k^2 \in \rho(H_{\varepsilon,y}), \quad \operatorname{Im} k > 0, \quad \varepsilon > 0, \quad y \in \mathbb{R}^3,\end{aligned} \tag{1.2.66}$$

where $A_\varepsilon(k)$, $B_\varepsilon(k) = \lambda(\varepsilon) W_2 G_{\varepsilon k} W_1$, $C_\varepsilon(k)$, $\varepsilon > 0$, are Hilbert–Schmidt operators with integral kernels

$$A_\varepsilon(k,x,x') = \int_{\mathbb{R}^3} d^3x''\, G_k(x - y - \varepsilon x'') W_1(x'', x'), \qquad \operatorname{Im} k > 0, \tag{1.2.67}$$

$$B_\varepsilon(k,x,x') = \lambda(\varepsilon) \int_{\mathbb{R}^6} d^3x''\, d^3x'''\, W_2(x,x'') G_{\varepsilon k}(x'' - x''') W_1(x''', x'), \qquad \operatorname{Im} k \ge 0, \tag{1.2.68}$$

$$C_\varepsilon(k,x,x') = \int_{\mathbb{R}^3} d^3x''\, W_2(x,x'') G_k(\varepsilon x'' + y - x'), \qquad \operatorname{Im} k > 0. \tag{1.2.69}$$

Similar to Lemma 1.2.2 we now have

Lemma 1.2.7. *Let $y \in \mathbb{R}^3$ and define rank-one operators $A(k)$, $C(k)$, and the Hilbert–Schmidt operator $W_2 G_0 W_1$ with integral kernels*

$$A(k, x, x') = G_k(x - y)\overline{v_1(x')}, \qquad \operatorname{Im} k > 0, \quad x \neq y, \tag{1.2.70}$$

$$(W_2 G_0 W_1)(x, x') = \int_{\mathbb{R}^6} d^3x''\, d^3x'''\, W_2(x, x'')(4\pi|x'' - x'''|)^{-1} W_1(x''', x'), \tag{1.2.71}$$

$$C(k, x, x') = u_2(x) G_k(y - x'), \qquad \operatorname{Im} k > 0, \quad x' \neq y, \tag{1.2.72}$$

where

$$v_1(x') = \int_{\mathbb{R}^3} d^3x\, \overline{W_1(x, x')}, \qquad u_2(x) = \int_{\mathbb{R}^3} d^3x'\, W_2(x, x'). \tag{1.2.73}$$

Then, for fixed k, $\operatorname{Im} k > 0$, $A_\varepsilon(k)$, $B_\varepsilon(k)$, $C_\varepsilon(k)$ converge in Hilbert–Schmidt norm to $A(k)$, $W_2 G_0 W_1$, $C(k)$, respectively, as $\varepsilon \downarrow 0$.

PROOF. Analogous to that of Lemma 1.2.2. ∎

Next we have to study zero-energy properties of H. If

$$W_2 G_0 W_1 \phi = -\phi \qquad \text{for some} \quad \phi \in L^2(\mathbb{R}^3) \tag{1.2.74}$$

we define

$$\psi(x) = (G_0 W_1 \phi)(x). \tag{1.2.75}$$

Then similar to Lemma 1.2.3 we obtain

Lemma 1.2.8. *Suppose $\tilde{\tilde{u}}_1, \tilde{\tilde{v}}_1 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Then $\psi \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$, $\nabla\psi \in L^2(\mathbb{R}^3)$, and $H\psi = 0$ in the sense of distributions. If, in addition, $|\cdot|^{1/2}\tilde{\tilde{u}}_1 \in L^1(\mathbb{R}^3)$, then $\psi \in L^2(\mathbb{R}^3)$ is equivalent to*

$$(v_1, \phi) = -\int_{\mathbb{R}^6} d^3x\, d^3x'\, W(x, x')\psi(x') = 0. \tag{1.2.76}$$

If $\psi \in L^2(\mathbb{R}^3)$, then $\psi \in H^{2,2}(\mathbb{R}^3)$ and $H\psi = 0$.

PROOF. As in Lemma 1.2.3, we decompose

$$\psi(x) = (4\pi|x|)^{-1}(v_1, \phi) + \psi_1(x), \tag{1.2.77}$$

where

$$\psi_1(x) = (4\pi)^{-1} \int_{\mathbb{R}^6} d^3x'\, d^3x''(|x - x'|^{-1} - |x|^{-1}) W_1(x', x'')\phi(x''). \tag{1.2.78}$$

Using (1.2.29) and (1.2.30) we get $\psi_1 \in L^2_{\mathrm{loc}}(\mathbb{R}^3)$ if $\tilde{\tilde{u}}_1 \in L^2(\mathbb{R}^3)$ and $\psi_1 \in L^2(\mathbb{R}^3)$ if

$|\cdot|^{1/2}\tilde{\tilde{u}}_1 \in L^1(\mathbb{R}^3)$. Similarly, one infers (cf. (1.2.32))

$$\int_{\mathbb{R}^3} d^3x\,|(\nabla\psi)(x)|^2 \le (4\pi)^{-2}\int_{\mathbb{R}^{12}} d^3x'\,d^3x''\,d^3y'\,d^3y''\,|W_1(x',x'')|\,|W_1(y',y'')|\cdot$$
$$\cdot|\phi(x'')|\,|\phi(y'')|\int_{\mathbb{R}^3} d^3x\,|x-x'|^{-2}|x-y'|^{-2}$$
$$\le (4\pi)^{-2}\,d\|\phi\|^2\int_{\mathbb{R}^6} d^3x'\,d^3y'\,\frac{\tilde{\tilde{u}}_1(x')\tilde{\tilde{u}}_1(y')}{|x'-y'|} < \infty \tag{1.2.79}$$

by Sobolev's inequality (cf. Lemma B.6). If $\psi \in L^2(\mathbb{R}^3)$, then by (1.2.79), $\psi \in H^{2,1}(\mathbb{R}^3)$ and hence ψ is in the form domain of H. The fact that $H\psi = 0$ in the sense of distributions then shows $\psi \in \mathscr{D}(H)$ and $H\psi = 0$. ∎

Zero-energy resonances (resp. zero-energy bound states) of H are now defined as before (i.e., one simply distinguishes whether $\psi \in L^2(\mathbb{R}^3)$ or not) assuming $\tilde{\tilde{u}}_1, \tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ and $|\cdot|^{1/2}\tilde{\tilde{u}}_1 \in L^1(\mathbb{R}^3)$. In particular, the case distinctions on page 20 apply with the only change that uG_0v should be replaced by $W_2G_0W_1$.

Lemma 1.2.4 then has to be replaced by

Lemma 1.2.9. *Let $\tilde{\tilde{u}}_1, \tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. In cases* II–IV *assume, in addition, $|\cdot|^{1/2}\tilde{\tilde{u}}_1 \in L^1(\mathbb{R}^3)$ and $\lambda'(0) \neq 0$ in cases* III *and* IV. *Then*

$$\text{n-}\lim_{\varepsilon\downarrow 0} \varepsilon[1 + B_\varepsilon(k)]^{-1} = \begin{cases} 0 & \text{in case I,} \\ [(4\pi)^{-1}ik|(v_1,\phi)|^2 + \lambda'(0)]^{-1}(\tilde{\phi},\cdot)\phi & \text{in case II,} \\ [\lambda'(0)]^{-1}\sum_{l=1}^{N}(\tilde{\phi}_l,\cdot)\phi_l & \text{in case III,} \\ \sum_{l,l'=1}^{N}(\tilde{\phi},B_1(k)\phi)_{ll'}^{-1}(\tilde{\phi}_{l'},\cdot)\phi_l & \text{in case IV,} \end{cases} \tag{1.2.80}$$

where $k^2 \in \mathbb{C} - \mathbb{R}$, $\operatorname{Im} k > 0$, *and $(\tilde{\phi}, B_1(k)\phi)_{ll'}^{-1}$ denotes the inverse of the matrix $(\tilde{\phi}_l, B_1(k)\phi_{l'})$*

$$W_2G_0W_1\phi_l = -\phi_l, \qquad W_1^*G_0W_2^*\tilde{\phi}_{l'} = -\tilde{\phi}_{l'},$$
$$(\tilde{\phi}_{l'},\phi_l) = -\delta_{ll'}, \qquad l, l' = 1,\ldots,N, \tag{1.2.81}$$
$$B_1(k) = \lambda'(0)W_2G_0W_1 + (4\pi)^{-1}ik(v_1,\cdot)u_2.$$

PROOF. One can follow the analogous proof of Lemma 1.2.4 step by step. ∎

Given Lemmas 1.2.7 and 1.2.9 we finally state

Theorem 1.2.10. *Let $\tilde{\tilde{u}}_1, \tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$, and $y \in \mathbb{R}^3$. In cases* II–IV *assume, in addition, $|\cdot|^{1/2}\tilde{\tilde{u}}_1 \in L^1(\mathbb{R}^3)$ and $\lambda'(0) \neq 0$ in cases* III *and* IV. *Then,* *if $k^2 \in \rho(-\Delta_{\alpha,y})$, we get $k^2 \in \rho(H_{\varepsilon,y})$ for $\varepsilon > 0$ small enough and that $H_{\varepsilon,y}$ converges to $-\Delta_{\alpha,y}$ in norm resolvent sense as $\varepsilon \downarrow 0$, viz.*

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}, \qquad y \in \mathbb{R}^3, \tag{1.2.82}$$

where α is given by

$$\alpha = \begin{cases} \infty & \textit{in case I}, \\ -\lambda'(0)|(v_1, \phi)|^{-2} & \textit{in case II}, \\ \infty & \textit{in case III}, \\ -\lambda'(0)\left\{\sum_{l=1}^{N} |(v_1, \phi_l)|^2\right\}^{-1} & \textit{in case IV}. \end{cases} \tag{1.2.83}$$

In particular, $H_{\varepsilon,y}$ converges in norm resolvent sense to $-\Delta$ in cases I *and* III *as $\varepsilon \downarrow 0$.*

PROOF. Identical to that of Theorem 1.2.5. ■

Clearly, our comments before Lemma 1.2.4 and after Lemma 1.2.3 and Theorem 1.2.5 apply as well for nonlocal interactions after a suitable reinterpretation. We omit the details.

To simplify the treatment in the following we assume from now on that

$$(v, \phi_1) \neq 0, \qquad (v, \phi_l) = 0, \qquad l = 2, \ldots, N, \quad \text{in case IV}. \tag{1.2.84}$$

While assumption (1.2.84) considerably reduces the complexity of the following proofs we emphasize that all results in Sects. 1.3, 1.4, and Ch. 2 immediately extend to the general situation $(v, \phi_1) \neq 0, \ldots, (v, \phi_M) \neq 0$, $(v, \phi_{M+1}) = 0, \ldots, (v, \phi_N) = 0$, $1 \leq M \leq N - 1$. (If V is spherically symmetric, then (1.2.84) automatically holds as explained before Lemma 1.2.4.)

I.1.3 Convergence of Eigenvalues and Resonances

Having proved norm resolvent convergence in Sect. 1.2, we now turn to the spectrum and investigate eigenvalues and resonances of $H_{\varepsilon,y}$ as $\varepsilon \downarrow 0$. Regarding the essential spectrum we note that Lemma 1.2.1 and Theorem B.1(b) imply

$$\sigma_{\text{ess}}(H_{\varepsilon,y}) = \sigma_{\text{ess}}(H_y(\varepsilon)) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3, \tag{1.3.1}$$

and by Theorem 1.1.4 this result remains true in the limit $\varepsilon \downarrow 0$,

$$\sigma_{\text{ess}}(-\Delta_{\alpha,y}) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3. \tag{1.3.2}$$

A detailed discussion of the discrete spectrum is given in

Theorem 1.3.1. *Let $y \in \mathbb{R}^3$ and assume $e^{2a|\cdot|}V \in R$ for some $a > 0$ is real-valued.*

(a) *In all cases* I–IV *any negative eigenvalue* $\tilde{E}_0 = \tilde{k}_0^2 < 0$ *of* $H = -\Delta \dotplus V$ *of multiplicity* M *gives rise to* M *(not necessarily distinct) negative eigenvalues* $E_{l,\varepsilon} = k_{l,\varepsilon}^2 < 0, l = 1, \ldots, M,$ *of* $H_{\varepsilon,y}$ *running to* $-\infty$ *as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon} = \varepsilon^{-1}\tilde{k}_0 + O(1), \qquad l = 1, \ldots, M. \tag{1.3.3}$$

In addition, $\varepsilon k_{l,\varepsilon}$ *is analytic in* ε *near* $\varepsilon = 0$.

(b) *Assume case* II. *If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ *with* $\alpha < 0$ *(i.e.,* $\lambda'(0) > 0$*), then* $-\Delta_{\alpha,y}$ *has the simple eigenvalue* $E_0 = k_0^2 < 0$, $k_0 = -4\pi i\alpha = 4\pi i\lambda'(0)|(v, \phi)|^{-2}$, *and the zero-energy resonance of* H *implies that for* $\varepsilon > 0$ *small enough* $H_{\varepsilon,y}$ *has precisely one simple eigenvalue* $E_\varepsilon = k_\varepsilon^2 < 0$ *near* E_0 *which is analytic in* ε *near* $\varepsilon = 0$

$$k_\varepsilon = k_0 + O(\varepsilon). \tag{1.3.4}$$

(c) *Assume case* III *and* $\lambda'(0) > 0$. *If* $N = 1$ *then the zero-energy bound state of* H *gives rise to a negative, simple eigenvalue* $E_{1,\varepsilon} = k_{1,\varepsilon}^2 < 0$ *of* $H_{\varepsilon,y}$ *running to* $-\infty$ *as* $\varepsilon \downarrow 0$ *like*

$$k_{1,\varepsilon} = \varepsilon^{-1/2} i \left\{ -8\pi\lambda'(0) \left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\tilde{\phi}_1(x)} v(x) \cdot \cdot |x - x'| v(x')\phi_1(x') \right]^{-1} \right\}^{1/2} + O(1). \tag{1.3.5}$$

(Note that $|x - x'|$ *is conditionally strictly negative* [298].*) In addition,* $\varepsilon^{1/2}k_{1,\varepsilon}$ *is analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$. *Moreover, if* $N > 1$, *let* c_l, $l = 1, \ldots, N$, *denote the eigenvalues (counting multiplicity) of the matrix* $(\tilde{\phi}_l, C\phi_{l'})$, $l, l' = 1, \ldots, N$, *where* C *is the Hilbert–Schmidt operator with kernel*

$$C(x, x') = -(8\pi)^{-1}u(x)|x - x'|v(x') \tag{1.3.6}$$

(necessarily, $c_l > 0, l = 1, \ldots, N$*). Then the zero-energy bound states of* H *give rise to* N *negative (not necessarily distinct) eigenvalues* $E_{l,\varepsilon} = k_{l,\varepsilon}^2 < 0$ *of* $H_{\varepsilon,y}$ *running to* $-\infty$ *as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon} = \varepsilon^{-1/2} i[\lambda'(0)/c_l]^{1/2} + O(1), \qquad l = 1, \ldots, N. \tag{1.3.7}$$

In addition, $\varepsilon^{1/2}k_{l,\varepsilon}$, $l = 1, \ldots, N$, *are analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ *(we choose* $\varepsilon^{1/2} > 0$ *for* $\varepsilon > 0$*) and the multiplicity of* $k_{l,\varepsilon}$ *coincides with that of the eigenvalue* c_l.

(d) *Assume case* IV *and* (1.2.84). *If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ *with* $\alpha < 0$ *(i.e.,* $\lambda'(0) > 0$*), then* $-\Delta_{\alpha,y}$ *has the simple eigenvalue* $E_0 = k_0^2 < 0, k_0 = -4\pi i\alpha = 4\pi i\lambda'(0)|(v, \phi_1)|^{-2}$, *and the zero-energy resonance of* H *implies that for* $\varepsilon > 0$ *small enough* $H_{\varepsilon,y}$ *has precisely one simple eigenvalue* $E_{1,\varepsilon} = k_{1,\varepsilon}^2 < 0$ *near* E_0 *which is analytic in* ε *near* $\varepsilon = 0$,

$$k_{1,\varepsilon} = k_0 + O(\varepsilon). \tag{1.3.8}$$

In addition, if $N = 2$, *the zero-energy bound state of* H *gives rise to a* *negative, simple eigenvalue* $E_{2,\varepsilon} = k_{2,\varepsilon}^2 < 0$ *of* $H_{\varepsilon,y}$ *running to* $-\infty$ *as* $\varepsilon \downarrow 0$ *like*

$$k_{2,\varepsilon} = \varepsilon^{-1/2} i \left\{ -8\pi\lambda'(0) \left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_2(x)} v(x) \cdot \right.\right.$$

$$\left.\left. \cdot |x - x'| v(x') \phi_2(x') \right]^{-1} \right\}^{1/2} + O(1), \qquad (1.3.9)$$

where $\varepsilon^{1/2} k_{2,\varepsilon}$ *is analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$.

For $N > 2$, *let again* c_l, $l = 1, \ldots, N$, *denote the eigenvalues (counting multiplicity) of the matrix* $(\tilde{\phi}_l, C\phi_{l'})$, $l, l' = 2, \ldots, N$ *(necessarily* $c_l > 0$, $l = 2, \ldots, N$*). Then the zero-energy bound states of H give rise to* $N - 1$ *negative (not necessarily distinct) eigenvalues* $E_{l,\varepsilon} = k_{l,\varepsilon}^2 < 0$ *of* $H_{\varepsilon,y}$ *running to* $-\infty$ *as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon} = \varepsilon^{-1/2} i [\lambda'(0)/c_l]^{1/2} + O(1), \qquad l = 2, \ldots, N, \qquad (1.3.10)$$

such that $\varepsilon^{1/2} k_{l,\varepsilon}$, $l = 2, \ldots, N$, *are analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ *(again* $\varepsilon^{1/2} > 0$ *for* $\varepsilon > 0$*) and the multiplicity of* $k_{l,\varepsilon}$ *coincides with that of* c_l.

PROOF. By eq. (1.2.16) and Theorem B.1(c), $H_{\varepsilon,y}$ has an eigenvalue $E_\varepsilon = k_\varepsilon^2 < 0$ if and only if -1 is an eigenvalue of $B_\varepsilon(k_\varepsilon)$.

(a) Let $\tilde{k} = \varepsilon k$ and define

$$B_{\varepsilon,\tilde{k}} = B_\varepsilon(\varepsilon^{-1}\tilde{k}) = \lambda(\varepsilon) u G_{\tilde{k}} v, \qquad \operatorname{Im} \tilde{k} \geq 0. \qquad (1.3.11)$$

By hypothesis, $B_{0,\tilde{k}_0}$ has an eigenvalue -1 and following the proof of expansion (1.2.42), $B_{\varepsilon,\tilde{k}}$ is easily seen to be analytic with respect to $(\varepsilon, \tilde{k})$ around $(0, \tilde{k}_0)$ in Hilbert–Schmidt norm. By the implicit function theorem and by Theorem B.2 the equation $\det_2(1 + B_{\varepsilon,\tilde{k}}) = 0$ has M (not necessarily distinct) solutions $\tilde{k}_{l,\varepsilon}$, $l = 1, \ldots, M$, for $|\varepsilon|$ small enough. Moreover, by scaling $x \to \varepsilon x$, $\varepsilon > 0$, and an additional translation $x \to x + y/\varepsilon$, $\varepsilon > 0$, $\tilde{k}_{l,\varepsilon}^2 < 0$, $l = 1, \ldots, M$, are the eigenvalues of $H(\varepsilon) = -\Delta \dotplus \lambda(\varepsilon) V$. An application of Rellich's theorem (cf. Lemma B.4) then proves analyticity of $\tilde{k}_{l,\varepsilon}$, $l = 1, \ldots, M$, in ε near $\varepsilon = 0$.

Of course, the same result follows directly from (degenerate) perturbation theory and the fact that due to the scaling property (1.2.11) the eigenvalues $E_\varepsilon = k_\varepsilon^2 < 0$ of $H_{\varepsilon,y}$ and $E(\varepsilon) = k(\varepsilon)^2 < 0$ of $H_y(\varepsilon)$ obey $k_\varepsilon = \varepsilon^{-1} k(\varepsilon)$.

(b) As in the proof of (1.2.42) $B_\varepsilon(k)$ is analytic with respect to (ε, k) in Hilbert–Schmidt norm near $\varepsilon = 0$ and any k with $\operatorname{Im} k > -a/\varepsilon_0$, $|\varepsilon| < \varepsilon_0$, and

$$B_\varepsilon(k) = [1 + \varepsilon\lambda'(0)] u G_0 v + (4\pi)^{-1} i\varepsilon k (v, \cdot) u + O(\varepsilon^2). \qquad (1.3.12)$$

Thus using [435]

$$\det_2(1 + A + B) = \det_2(1 + A) \det[1 + (1 + A)^{-1} B] e^{-\operatorname{Tr} B}, \qquad (1.3.13)$$

if $A \in \mathscr{B}_2(\mathscr{H})$, $(1 + A)^{-1} \in \mathscr{B}(\mathscr{H})$, $B \in \mathscr{B}_1(\mathscr{H})$ for some (separable) Hilbert space $\mathscr{H}$, we obtain that

$$\det_2[1 + B_\varepsilon(k)] = \det_2[1 + B_\varepsilon(k) + P] \det\{1 - [1 + B_\varepsilon(k) + P]^{-1} P\} e, \quad (1.3.14)$$

since

$$[1 + uG_0 v + P]^{-1} = P + T, \qquad P = -(\tilde{\phi}, \cdot)\phi \qquad (1.3.15)$$

exists. Consequently, for $|\varepsilon|$ small enough,

$$\det{}_2[1 + B_\varepsilon(k)] = 0 \quad \text{iff}$$
$$\det\{1 - [1 + B_\varepsilon(k) + P]^{-1}P\} = 1 - (\tilde{\phi}, [1 + B_\varepsilon(k) + P]^{-1}\phi) = 0. \tag{1.3.16}$$

From the expansion (1.3.12) we get

$$[1 + B_\varepsilon(k) + P]^{-1} = (1 + uG_0v + P)^{-1} - \varepsilon(1 + uG_0v + P)^{-1} \cdot \\ \cdot [(ik/4\pi)(v, \cdot)u + \lambda'(0)uG_0v](1 + uG_0v + P)^{-1} + O(\varepsilon^2), \tag{1.3.17}$$

and hence by (1.3.15)

$$P[1 + B_\varepsilon(k) + P]^{-1}P = -(\tilde{\phi}, \cdot)\phi - \varepsilon(ik/4\pi)|(v, \phi)|^2(\tilde{\phi}, \cdot)\phi - \varepsilon\lambda'(0)(\tilde{\phi}, \cdot)\phi + O(\varepsilon^2). \tag{1.3.18}$$

Insertion of (1.3.18) into (1.3.16) and the implicit function theorem immediately yield all assertions of part (b) since (1.3.16) has a simple zero at $(\varepsilon, k) = (0, k_0)$, $k_0 = 4\pi i\lambda'(0)|(v, \phi)|^{-2}$.

(c) We introduce

$$\mu = \varepsilon^{1/2}, \qquad \tilde{k} = \varepsilon^{1/2}k. \tag{1.3.19}$$

Then

$$1 + B_\varepsilon(k) = 1 + \tilde{B}_\mu(\tilde{k}) = 1 + \lambda(\mu^2)uG_{\mu\tilde{k}}v \\ = 1 + uG_0v + \mu(i\tilde{k}/4\pi)(v, \cdot)u + \mu^2\lambda'(0)uG_0v + \mu^2\tilde{k}^2C + O(\mu^3), \tag{1.3.20}$$

where C is defined by (1.3.6), and $\tilde{B}_\mu(\tilde{k})$ is analytic in Hilbert–Schmidt norm with respect to μ and $\tilde{k}$ for $|\mu|$ small enough and $\operatorname{Im}\tilde{k} > -a/\mu_0$, $|\mu| < \mu_0$. Consequently,

$$\det{}_2[1 + \tilde{B}_\mu(\tilde{k})] = \det{}_2[1 + B_\mu(\tilde{k}) + P]\det{}_2\{1 - [1 + B_\mu(\tilde{k}) + P]^{-1}P\} \tag{1.3.21}$$

implies, for $|\mu|$ small enough, that

$$\det{}_2\{1 - [1 + B_\mu(\tilde{k}) + P]^{-1}P\} = 0 \tag{1.3.22}$$

since

$$[1 + uG_0v + P]^{-1} = P + T \tag{1.3.23}$$

exists. Moreover, the fact that

$$\det{}_2(1 + A) = \det(1 + A)\exp[-\operatorname{Tr}(A)] \tag{1.3.24}$$

for $A \in \mathscr{B}_1(\mathscr{H})$ ($\mathscr{H}$ a separable Hilbert space) shows that for $|\mu|$ small enough (1.3.22) is equivalent to

$$\det\{1 - [1 + B_\mu(\tilde{k}) + P]^{-1}P\} = \det\{1 - P[1 + B_\mu(\tilde{k}) + P]^{-1}P\} = 0. \tag{1.3.25}$$

Since P is of finite rank, (1.3.25) is analytic with respect to μ, $\tilde{k}$ for $|\mu| < \mu_0$ small enough and $\operatorname{Im}\tilde{k} > -a/\mu_0$ [261]. From the expansion (1.3.20) we infer that

$$[1 + B_\mu(\tilde{k}) + P]^{-1} \\ = (1 + uG_0v + P)^{-1} - \mu(i\tilde{k}/4\pi)(1 + uG_0v + P)^{-1}(v, \cdot)u(1 + uG_0v + P)^{-1} \\ - \mu^2\lambda'(0)(1 + uG_0v + P)^{-1}uG_0v(1 + uG_0v + P)^{-1} \\ - \mu^2\tilde{k}^2(1 + uG_0v + P)^{-1}C(1 + uG_0v + P)^{-1} \\ - \mu^2(\tilde{k}/4\pi)^2[(1 + uG_0v + P)^{-1}(v, \cdot)u]^2(1 + uG_0v + P)^{-1} + O(\mu^3) \tag{1.3.26}$$

and hence using (1.3.23) and $Pu = 0$

$$P[1 + B_\mu(\tilde{k}) + P]^{-1}P = [1 + \mu^2\lambda'(0)]P - \mu^2\tilde{k}^2PCP + O(\mu^3). \quad (1.3.27)$$

From (1.3.25) and (1.3.27) we obtain

$$\det\{1 - P[1 + \lambda'(0)\mu^2 - \mu^2\tilde{k}^2C]P\} = O(\mu) \quad (1.3.28)$$

and thus

$$\det\{\lambda'(0)\tilde{k}^{-2}\delta_{ll'} + (\tilde{\phi}_{l'}C\phi_{l'})\} = O(\mu). \quad (1.3.29)$$

From the fact that [272]

$$(\tilde{\phi}_l, C\phi_{l'}) = \int_{\mathbb{R}^3} d^3p\,|p|^{-4}\overline{(v\phi_l)^\wedge(p)}\,(v\phi_{l'})^\wedge(p) \equiv \langle\phi_l, \phi_{l'}\rangle, \qquad l, l' = 1, \ldots, N, \quad (1.3.30)$$

which follows from $(v\phi_l)^\wedge \in C^\infty(\mathbb{R}^3)$ and $(v\phi_l)^\wedge(0) = 0$, $l = 1, \ldots, N$ (since $e^{a|\cdot|}v\phi_l \in L^1(\mathbb{R}^3)$ for some $a > 0$ and $(v, \phi_l) = 0$, $l = 1, \ldots, N$) one can show that the self-adjoint matrix $\langle\phi_l, \phi_{l'}\rangle$, $l, l' = 1, \ldots, N$, is positive definite. In fact,

$$\sum_{l,l'=1}^{N} \langle\phi_l, \phi_{l'}\rangle\bar{\xi}_l\xi_{l'} = \left\langle \sum_{l=1}^{N} \xi_l\phi_l, \sum_{l'=1}^{N} \xi_{l'}\phi_{l'} \right\rangle > 0, \qquad \xi \in \mathbb{C}^N - \{0\}, \quad (1.3.31)$$

since $\{\phi_l\}$, $\{(v\phi_l)^\wedge\}$ and hence the vectors $\{[|\cdot|^{-2}(v\phi_l)]^\wedge\}$, $l = 1, \ldots, N$, are linearly independent. Denote by c_l, $l = 1, \ldots, N$, the eigenvalues of $(\tilde{\phi}_l, C\phi_{l'})$ (counting multiplicity). Then to zeroth order in μ, (1.3.29) has the solutions

$$\tilde{k}_{l,0}^{\pm} = \pm i(\lambda'(0)/c_l)^{1/2}, \qquad l = 1, \ldots, N. \quad (1.3.32)$$

If in (1.3.19) we use the principal branch for $\varepsilon^{1/2}$ (i.e., $\varepsilon^{1/2} > 0$ for $\varepsilon > 0$) then the plus sign has to be chosen in (1.3.32). To prove that (1.3.29) has solutions $\tilde{k}_{l,\mu}$ analytic in μ we argue as follows. By repeating the calculations leading to (1.3.29) but keeping $\lambda(\mu^2)$ fixed and only expanding with respect to the variable β

$$\beta = i\mu\tilde{k}, \quad (1.3.33)$$

we obtain

$$\det\left\{\frac{\lambda(\mu^2) - 1}{\mu^2\tilde{k}^2}\mu^2\tilde{k}^2\delta_{ll'} - (\mu i\tilde{k})^2(\tilde{\phi}_l, C\phi_{l'}) + \sum_{r=3}^{\infty}(\mu i\tilde{k})^r\Phi_{r,ll'}\right\} = 0. \quad (1.3.34)$$

Introducing

$$\nu = [\lambda(\mu^2) - 1]/\mu^2\tilde{k}^2 \quad (1.3.35)$$

as another new variable, (1.3.34) is equivalent to

$$\det\left\{\nu\delta_{ll'} + (\tilde{\phi}_l, C\phi_{l'}) + \sum_{r=1}^{\infty}\beta^r\Phi_{r+2,ll'}\right\} = 0. \quad (1.3.36)$$

By inspection $\Phi_{r,ll'}$ is a self-adjoint matrix and $\beta \in \mathbb{R}$ for $\mu \in \mathbb{R}$ and $\tilde{k} \in i\mathbb{R}$. Consequently, we can apply Rellich's theorem (cf. Lemma B.4) and obtain ν_l as an analytic function of β

$$\nu_l(\beta) = -c_l + O(\beta), \qquad l = 1, \ldots, N. \quad (1.3.37)$$

Since $c_l \neq 0$ we get

$$\tilde{k}_l^2(\beta, \mu) = -c_l^{-1}\sum_{q=1}^{\infty}(q!)^{-1}\lambda^{(q)}(0)\mu^{2q-2} + \sum_{r=1}^{\infty}\alpha_r\beta^r\sum_{q=1}^{\infty}(q!)^{-1}\lambda^{(q)}(0)\mu^{2q-2}, \quad (1.3.38)$$

or

$$\tilde{k}_l^2 = -c_l^{-1} \sum_{q=1}^{\infty} (q!)^{-1} \lambda^{(q)}(0) \mu^{2q-2} + \sum_{r=1}^{\infty} \alpha_r(\mu i \tilde{k}_l)^r \sum_{q=1}^{\infty} (q!)^{-1} \lambda^{(q)}(0) \mu^{2q-2},$$

$$l = 1, \ldots, N. \quad (1.3.39)$$

Introducing

$$F_l(x, \mu) = -x^2 - c_l^{-1} \sum_{q=1}^{\infty} (q!)^{-1} \lambda^{(q)}(0) \mu^{2q-2} + \sum_{r=1}^{\infty} \alpha_r(\mu i x)^r \sum_{q=1}^{\infty} (q!)^{-1} \lambda^{(q)}(0) \mu^{2q-2},$$

$$l = 1, \ldots, N, \quad (1.3.40)$$

we infer that $F_l(\cdot, \cdot)$ is analytic near $(\tilde{k}_{l,0}^+, 0)$ with

$$F_l(\tilde{k}_{l,0}^+, 0) = 0, \qquad \frac{\partial}{\partial x} F_l(x, \mu)|_{(\tilde{k}_{l,0}^+, 0)} \neq 0. \tag{1.3.41}$$

By the implicit function theorem one can solve for x as an analytic function of μ.

(d) In order to determine the effect of the zero-energy bound state of H we define

$$P' = -\sum_{l=2}^{N} (\tilde{\phi}_l, \cdot)\phi_l, \qquad P_1 = -(\tilde{\phi}_1, \cdot)\phi_1 \tag{1.3.42}$$

and note that similar to (1.2.36)

$$(1 + uG_0 v + P' + z)^{-1} = z^{-1} P_1 + \sum_{m=0}^{\infty} (-z)^m T_1^{m+1}, \qquad z \in \mathbb{C} - \{0\} \text{ small enough} \tag{1.3.43}$$

using that -1 is a simple eigenvalue of $uG_0 v + P'$, where

$$T_1 = \operatorname*{n-lim}_{z \to 0} (1 + uG_0 v + P' + z)^{-1}[1 - P_1] \tag{1.3.44}$$

and

$$P'T_1 = T_1 P' = P'T_1 P' = P', \qquad P_1 T_1 = 0. \tag{1.3.45}$$

Next we prove that $[1 + B_\mu(\tilde{k}) + P']^{-1}P'$ is analytic in μ and $\tilde{k}$ for $|\mu|$ small enough and $\operatorname{Im} \tilde{k} > -a/\mu_0$, $|\mu| < \mu_0$. In fact, using the expansions (1.3.20) and (1.3.43) and the relations (1.3.45) one obtains along the lines of (1.2.45) that

$$[1 + B_\mu(\tilde{k}) + P']^{-1}P' = \{1 - P_1 + (ik/4\pi)P_1(v, \cdot)u + O(\mu)\}^{-1}[P' + O(\mu)] \tag{1.3.46}$$

is analytic in μ near $\mu = 0$ since $[1 - P_1 + (ik/4\pi)P_1(v, \cdot)u]^{-1}$ is easily shown to exist by a straightforward application of the formula

$$[1 + \beta(\tilde{\psi}, \cdot)\psi + R]^{-1} = [1 + R]^{-1} - \{\beta^{-1} + (\tilde{\psi}, [1 + R]^{-1}\psi)\}^{-1} \cdot$$
$$\cdot([1 + R^*]^{-1}\tilde{\psi}, \cdot)[1 + R]^{-1}\psi \tag{1.3.47}$$

assuming $\beta \in \mathbb{C}$, $\tilde{\psi}, \psi \in \mathscr{H}$, $R, [1 + R]^{-1} \in \mathscr{B}(\mathscr{H})$, $\{\beta^{-1} + (\tilde{\psi}, [1 + R]^{-1}\psi)\} \neq 0$ for some separable Hilbert space $\mathscr{H}$. From now on one can follow the proof of part (c) step by step after replacing P by P'. Equation (1.3.27) then reads

$$P'[1 + B_\mu(\tilde{k}) + P']^{-1}P' = [1 + \mu^2 \lambda'(0)]P' - \mu^2 \tilde{k}^2 P'CP' + O(\mu^3), \tag{1.3.48}$$

which proves the assertions in connection with (1.3.9) and (1.3.10). It remains to determine the contribution of the zero-energy resonance of H. First of all, we note that

$$[1 + B_\varepsilon(k) + P_1]^{-1}P_1 = \{1 - [1 + \lambda'(0)]P' + O(\varepsilon)\}^{-1}[P_1 + O(\varepsilon)] \quad (1.3.49)$$

is analytic in ε near $\varepsilon = 0$ since

$$\{1 - [1 + \lambda'(0)]P'\}^{-1} = 1 - [\lambda'(0)]^{-1}[1 + \lambda'(0)]P' \quad (1.3.50)$$

exists because of the assumption $\lambda'(0) \neq 0$. Consequently, we get

$$1 + B_\varepsilon(k) = [1 + B_\varepsilon(k) + P_1]\{1 - [1 + B_\varepsilon(k) + P_1]^{-1}P_1\}, \quad (1.3.51)$$

and since (cf. (1.3.18))

$$\begin{aligned} P_1[1 + B_\varepsilon(k) + P_1]^{-1}P_1 = {} & -(\tilde{\phi}_1, \cdot)\phi_1 - \varepsilon(ik/4\pi)|(v, \phi_1)|^2(\tilde{\phi}_1, \cdot)\phi_1 \\ & - \varepsilon\lambda'(0)(\tilde{\phi}_1, \cdot)\phi_1 + O(\varepsilon^2), \end{aligned} \quad (1.3.52)$$

one can follow the last part of the proof of (b) step by step. ■

Next we derive similar results for *resonances*. We first recall the one-to-one correspondence between a negative bound state $E_0 = k_0^2 < 0$ of some Hamiltonian $H = -\Delta \dotplus V$, $V \in R$ real-valued, and a pole of $(1 + uG_k v)^{-1}$ at $k_0 = i\sqrt{-E_0}$ in the upper k-plane. In particular, the multiplicity of E_0 coincides with the (geometric) multiplicity of the eigenvalue -1 of $uG_{k_0}v$ and also coincides with the multiplicity of the zero of the modified Fredholm determinant $\det_2(1 + uG_k v)$ at $k = k_0$ (cf. Appendix B). If $V \in R$, then $uG_k v$ is holomorphic in Hilbert–Schmidt norm with respect to k in $\operatorname{Im} k > 0$. In order to define resonances we now assume that $uG_k v$ has an analytic continuation into the region $0 > \operatorname{Im} k > -a$ for some $a > 0$ such that $uG_k v$ remains Hilbert–Schmidt for $0 \geq \operatorname{Im} k > -a$. In this case k_1 with $0 > \operatorname{Im} k_1 > -a$ is called a resonance of H if $uG_{k_1}v$ has an eigenvalue -1. Similarly, the multiplicity of the resonance k_1 is defined to be the multiplicity of the zero of the modified Fredholm determinant $\det_2(1 + uG_k v)$ at $k = k_1$ (c.f. Appendix B).

Resonances for the point interaction Hamiltonian $-\Delta_{\alpha,y}$ are defined analogously as poles of the resolvent kernel $(-\Delta_{\alpha,y} - k^2)^{-1}(x, x')$, $x \neq x'$, $x \neq y$, $x' \neq y$ in the lower k-plane. According to this definition $-\Delta_{\alpha,y}$ has a simple resonance k_1 if and only if $\alpha \geq 0$ in which case

$$k_1 = -4\pi i\alpha, \qquad \psi_{k_1}(x) = e^{4\pi\alpha|x-y|}/|x - y|, \qquad x \neq y, \quad \alpha \geq 0, \quad (1.3.53)$$

with ψ_{k_1} being the corresponding resonance function. The origin $k = 0$ needs a separate discussion: In fact, as discussed in detail in Sect. 1.2, $k = 0$ can be resonance and/or a bound state of $H = -\Delta \dotplus V$. For $\alpha = 0$ the operator $-\Delta_{\alpha,y}$ has only a zero-energy resonance and no zero-energy bound state.

The analog of Theorem 1.3.1 for resonances now reads

Theorem 1.3.2. *Let $y \in \mathbb{R}^3$ and assume that $e^{2a|\cdot|}V \in R$ for all $a > 0$ is real-valued.*

(a) *In all cases* I–IV *any resonance $\tilde{k}_0$, $\operatorname{Im} \tilde{k}_0 < 0$, of $H = -\Delta \dotplus V$ of multiplicity M gives rise to M (not necessarily distinct) resonances $k_{l,\varepsilon}$,*

$\operatorname{Im} k_{l,\varepsilon} < 0$, $l = 1, \ldots, m$, of $H_{\varepsilon,y}$ running to infinity as $\varepsilon \downarrow 0$ like

$$k_{l,\varepsilon} = \varepsilon^{-1}\tilde{k}_0 + O(\varepsilon^{(1-m_l)/m_l}), \qquad m_l \geq 1, \quad l = 1, \ldots, m, \quad (1.3.54)$$

where $\varepsilon k_{l,\varepsilon}$ have convergent Puiseux expansions near $\varepsilon = 0$, i.e., there exist functions h_l analytic near the origin, $h_l(0) = 0$, $l = 1, \ldots, m$, such that

$$\varepsilon k_{l,\varepsilon} = \tilde{k}_0 + h_l(\varepsilon^{1/m_l}) = \tilde{k}_0 + \sum_{r=1}^{\infty} a_{l,r}\varepsilon^{r/m_l},$$

$$m_l \geq 1, \quad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M. \quad (1.3.55)$$

(b) *Assume case* II. *If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ *with* $\alpha > 0$ *(i.e.,* $\lambda'(0) < 0$*), then* $-\Delta_{\alpha,y}$ *has the simple resonance* $k_0 = -4\pi i\alpha = 4\pi i\lambda'(0)|(v, \phi)|^{-2}$ *and the zero-energy resonance of H implies that for $\varepsilon > 0$ small enough $H_{\varepsilon,y}$ has precisely one simple resonance k_ε, $\operatorname{Im} k_\varepsilon < 0$, $\operatorname{Re} k_\varepsilon = 0$, near k_0 which is analytic in ε near $\varepsilon = 0$ and hence fulfills* (1.3.4).

(c) *Assume case* III. *If $\lambda'(0) > 0$ and $N = 1$ the zero-energy bound state of H gives rise to a simple resonance $k_{1,\varepsilon}^-$ $\operatorname{Im} k_{1,\varepsilon}^- < 0$, $\operatorname{Re} k_{1,\varepsilon}^- = 0$, of $H_{\varepsilon,y}$ running to infinity as $\varepsilon \downarrow 0$ like*

$$k_{1,\varepsilon}^- = -i\varepsilon^{-1/2}\left\{-8\pi\lambda'(0)\left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_1(x)}v(x)\cdot \cdot|x - x'|v(x')\phi_1(x')\right]^{-1}\right\}^{1/2} + O(1) \quad (1.3.56)$$

such that $\varepsilon^{1/2}k_{1,\varepsilon}^-$ is analytic in $\varepsilon^{1/2}$ near $\varepsilon^{1/2} = 0$ (we choose $\varepsilon^{1/2} > 0$ for $\varepsilon > 0$).

If $\lambda'(0) < 0$ and $N = 1$ the zero-energy bound state of H gives rise to a resonance pair $k_{1,\varepsilon}^{\pm}$ of $H_{\varepsilon,y}$ (both resonances are simple) running to infinity as $\varepsilon \downarrow 0$ like

$$k_{1,\varepsilon}^{\pm} = \pm\varepsilon^{-1/2}\left\{8\pi\lambda'(0)\left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_1(x)}v(x)\cdot \cdot|x - x'|v(x')\phi_1(x')\right]^{-1}\right\}^{1/2} + O(1) \quad (1.3.57)$$

such that $\varepsilon^{1/2}k_{1,\varepsilon}^{\pm}$ are analytic in $\varepsilon^{1/2}$ near $\varepsilon^{1/2} = 0$.

If $\lambda'(0) > 0$ and $N > 1$ the zero-energy bound states of H give rise to N (not necessarily distinct) resonances $k_{l,\varepsilon}^-$, $\operatorname{Im} k_{l,\varepsilon}^- < 0$, $\operatorname{Re} k_{l,\varepsilon}^- = 0$, $l = 1, \ldots, N$, of $H_{\varepsilon,y}$ running to infinity as $\varepsilon \downarrow 0$ like

$$k_{l,\varepsilon}^- = -\varepsilon^{-1/2}i[\lambda'(0)/c_{l'}]^{1/2} + O(1), \qquad l = 1, \ldots, N, \quad (1.3.58)$$

with $c_l > 0$ the eigenvalues of $(\tilde{\phi}_l, C\phi_{l'})$, $l, l' = 1, \ldots, N$. Again $\varepsilon^{1/2}k_{l,\varepsilon}^-$, $l = 1, \ldots, N$, are analytic in $\varepsilon^{1/2}$ near $\varepsilon^{1/2} = 0$ and the multiplicity of $k_{l,\varepsilon}^-$ coincides with that of the eigenvalue c_l. If $\lambda'(0) < 0$ and $N > 1$ the zero-energy bound states of H give rise to N (not necessarily distinct) *resonance pairs* $k_{l,\varepsilon}^{\pm}$, $l = 1, \dots, N$, *of* $H_{\varepsilon,y}$ *running to infinity as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon}^{\pm} = \pm\varepsilon^{-1/2}[-\lambda'(0)/c_l]^{1/2} + O(1), \qquad l = 1, \dots, N. \quad (1.3.59)$$

Each $\varepsilon^{1/2}k_{l,\varepsilon}^{\pm}$, $l = 1, \dots, N$, *is analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ *and the multiplicity of* $k_{l,\varepsilon}^{\pm}$ *coincides with that of* c_l.

(d) *Assume case* IV *and* (1.2.84). *If* n-$\lim_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ *with* $\alpha > 0$ (*i.e.*, $\lambda'(0) < 0$) *then* $-\Delta_{\alpha,y}$ *has the simple resonance* $k_0 = -4\pi i\alpha = 4\pi i\lambda'(0)|(v, \phi_1)|^{-2}$ *and the zero-energy resonance of* H *implies that for* $\varepsilon > 0$ *small enough* $H_{\varepsilon,y}$ *has precisely one simple resonance* $k_{1,\varepsilon}$, $\operatorname{Im} k_{1,\varepsilon} < 0$, $\operatorname{Re} k_{1,\varepsilon} = 0$ near k_0 *which is analytic in* ε *near* $\varepsilon = 0$ *and hence satisfies* (1.3.8).

If $\lambda'(0) > 0$ *and* $N = 2$ *the zero-energy bound state of* H *gives rise to a simple resonance* $k_{2,\varepsilon}^{-}$, $\operatorname{Im} k_{2,\varepsilon}^{-} < 0$, $\operatorname{Re} k_{2,\varepsilon}^{-} = 0$, *of* $H_{\varepsilon,y}$ *running to infinity as* $\varepsilon \downarrow 0$ *like*

$$k_{2,\varepsilon}^{-} = -i\varepsilon^{-1/2}\left\{-8\pi\lambda'(0)\left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_2(x)}v(x)\cdot \cdot|x - x'|v(x')\phi_2(x')\right]^{-1}\right\}^{1/2} + O(1), \quad (1.3.60)$$

such that $\varepsilon^{1/2}k_{2,\varepsilon}^{-}$ *is analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ (*again* $\varepsilon^{1/2} > 0$ *for* $\varepsilon > 0$).

If $\lambda'(0) < 0$ *and* $N = 2$ *the zero-energy bound state of* H *gives rise to a resonance pair* $k_{2,\varepsilon}^{\pm}$ *of* $H_{\varepsilon,y}$ (*both resonances are simple*) *running to infinity as* $\varepsilon \downarrow 0$ *like*

$$k_{2,\varepsilon}^{\pm} = \pm\varepsilon^{-1/2}\left\{8\pi\lambda'(0)\left[\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_2(x)}v(x)\cdot \cdot|x - x'|v(x')\phi_2(x')\right]^{-1}\right\}^{1/2} + O(1), \quad (1.3.61)$$

where $\varepsilon^{1/2}k_{2,\varepsilon}^{\pm}$ *are analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$.

If $\lambda'(0) > 0$ *and* $N > 2$ *the zero-energy bound state of* H *gives rise to* $N - 1$ (*not necessarily distinct*) *resonances* $k_{l,\varepsilon}^{-}$, $\operatorname{Im} k_{l,\varepsilon}^{-} < 0$, $\operatorname{Re} k_{l,\varepsilon}^{-} = 0$, $l = 2, \dots, N$, *of* $H_{\varepsilon,y}$ *running to infinity as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon}^{-} = -\varepsilon^{-1/2}i[\lambda'(0)/c_l]^{1/2} + O(1), \qquad l = 1, \dots, N, \quad (1.3.62)$$

with $c_l > 0$ *the eigenvalues of* $(\tilde{\phi}_l, C\phi_{l'})$, $l, l' = 2, \dots, N$. *Again* $\varepsilon^{1/2}k_{l,\varepsilon}^{-}$, $l = 2, \dots, N$, *are analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ *and the multiplicity of* $k_{l,\varepsilon}^{-}$ *coincides with that of* c_l.

If $\lambda'(0) < 0$ *and* $N > 2$ *the zero-energy bound state of* H *gives rise to* $N - 1$ (*not necessarily distinct*) *resonance pairs* $k_{l,\varepsilon}^{\pm}$, $l = 2, \dots, N$, *of* $H_{\varepsilon,y}$ *running to infinity as* $\varepsilon \downarrow 0$ *like*

$$k_{l,\varepsilon}^{\pm} = \pm\varepsilon^{-1/2}[-\lambda'(0)/c_l]^{1/2} + O(1), \qquad l = 2, \dots, N. \quad (1.3.63)$$

In addition, each $\varepsilon^{1/2}k_{l,\varepsilon}^{\pm}$, $l = 2, \dots, N$, *is analytic in* $\varepsilon^{1/2}$ *near* $\varepsilon^{1/2} = 0$ *and the multiplicity of* $k_{l,\varepsilon}^{\pm}$ *coincides with that of* c_l.

PROOF. (a) Here one can follow the proof of Theorem 1.3.1(a) step by step. The only difference concerns the fact that now, in general, there is no constraint $m_l = 1$.

(b)–(d). All considerations about antibound states (i.e., resonances on the negative imaginary axis) follow directly from the proof of Theorem 1.3.1(b)–(d) since one can again apply Rellich's theorem. The conclusions about the resonance pairs are obtained as follows: By (1.2.11) every (anti-) bound state $k_{l,\varepsilon}$ of $H_{\varepsilon,y}$ corresponds to an (anti-) bound state $k_l(\varepsilon) = \varepsilon k_{l,\varepsilon}$ of $H_y(\varepsilon)$. Moreover, since $k_{l,\varepsilon} = O(\varepsilon^{-1/2})$ as $\varepsilon \downarrow 0$, $k_l(\varepsilon) = O(\varepsilon^{1/2})$ runs to zero as $\varepsilon \downarrow 0$. In fact, at $\varepsilon = 0$ the bound state and antibound state collide. In other words, for $\varepsilon > 0$, $\lambda'(0) > 0$ the solutions $k_l(\varepsilon)$ of the equation $\det_2[1 + \tilde{B}(\varepsilon, k)] = 0$ (cf. (1.3.7)) have a square root branch point at $\varepsilon = 0$,

$$k_l^{\pm}(\varepsilon) = \pm i|\varepsilon|^{1/2}[\lambda'(0)/c_l]^{1/2} + O(\varepsilon). \tag{1.3.64}$$

For $\lambda'(0) < 0$, or equivalently for $\varepsilon < 0$, we then get the resonance pair

$$k_l^{\pm}(\varepsilon) = \pm |\varepsilon|^{1/2}[-\lambda'(0)/c_l]^{1/2} + O(\varepsilon). \tag{1.3.65}$$

■

We note that if $\lambda'(0) = 0$ in case II then the same analysis shows that $k_\varepsilon = O(\varepsilon)$ as $\varepsilon \downarrow 0$. It then depends on the first nonvanishing coefficient in the Taylor expansion of k_ε whether $\operatorname{Im} k_\varepsilon \gtrless 0$ and hence whether $H_{\varepsilon,y}$ has a simple bound state or a resonance.

I.1.4 Stationary Scattering Theory

In this section we discuss scattering theory in connection with point interactions and prove that scattering quantities corresponding to $H_{\varepsilon,y}$ converge in a reasonable sense to that of the point interaction Hamiltonian $-\Delta_{\alpha,y}$ as $\varepsilon \downarrow 0$.

We first treat stationary scattering theory for the pair $(-\Delta_{\alpha,y}, -\Delta)$. Since $-\Delta_{\alpha,y}$ is invariant under rotations in $\mathbb{R}^3$ with center y we first concentrate on the partial wave decomposition (1.1.15). The fact that $-\Delta_{\alpha,y}$ actually describes an *s-wave interaction* (since the partial wave decompositions of $-\Delta_{\alpha,y}$ and the kinetic energy operator $-\Delta$ coincide for $l \geq 1$) considerably reduces the problem. Henceforth, we mainly confine ourselves to the case $l = 0$.

Define

$$\psi_{0,\alpha}(k, r) = k^{-1} \sin kr + (4\pi\alpha - ik)^{-1} e^{ikr}, \qquad k \geq 0, \quad -\infty < \alpha \leq \infty, \quad r \geq 0. \tag{1.4.1}$$

Then by inspection

$$\begin{aligned} &-4\pi\alpha\psi_{0,\alpha}(k, 0+) + \psi'_{0,\alpha}(k, 0+) = 0, \\ &-\psi''_{0,\alpha}(k, r) = k^2\psi_{0,\alpha}(k, r), \qquad r > 0, \\ &\lim_{\varepsilon\downarrow 0} \lim_{r'\to\infty} e^{-i(k+i\varepsilon)r'}[h_{0,\alpha} - (k + i\varepsilon)^2]^{-1}(r, r') = \psi_{0,\alpha}(k, r), \qquad r \geq 0; \\ &\qquad\qquad k \geq 0, \quad -\infty < \alpha \leq \infty. \end{aligned} \tag{1.4.2}$$

Hence $\psi_{0,\alpha}(k)$ constitute a set of generalized eigenfunctions ([353], Ch. VI) associated with $h_{0,\alpha}$. Similarly,

$$\psi_l(k, r) = (\pi r/2k)^{1/2} J_{l+1/2}(kr), \qquad k, r \geq 0, \quad l = 1, 2, \ldots, \tag{1.4.3}$$

are generalized eigenfunctions of $\dot{h}_l$, $l = 1, 2, \ldots$, where $J_\nu(\cdot)$ denote Bessel functions of order ν [1]. By introducing the *s-wave scattering phase shift* $\boldsymbol{\delta}_{0,\alpha}(k)$ via

$$\cos[\boldsymbol{\delta}_{0,\alpha}(k)] = 4\pi\alpha[(4\pi\alpha)^2 + k^2]^{-1/2}, \qquad \sin[\boldsymbol{\delta}_{0,\alpha}(k)] = k[(4\pi\alpha)^2 + k^2]^{-1/2},$$
$$k \geq 0, \quad -\infty < \alpha \leq \infty, \tag{1.4.4}$$

the expression (1.4.1) can be rewritten in the familiar form

$$\psi_{0,\alpha}(k, r) = k^{-1} e^{i\boldsymbol{\delta}_{0,\alpha}(k)} \sin[kr + \boldsymbol{\delta}_{0,\alpha}(k)], \qquad k > 0, \quad -\infty < \alpha \leq \infty, \quad r \geq 0. \tag{1.4.5}$$

In particular, from (1.4.3) and (1.4.4) one derives the (on-shell) *partial wave scattering matrix*

$$\mathscr{S}_{0,\alpha}(k) = e^{2i\boldsymbol{\delta}_{0,\alpha}(k)} = (4\pi\alpha - ik)^{-1}(4\pi\alpha + ik), \qquad k \geq 0, \quad -\infty < \alpha \leq \infty,$$
$$\mathscr{S}_l(k) = 1, \qquad \boldsymbol{\delta}_l(k) = 0, \quad l = 1, 2, \ldots. \tag{1.4.6}$$

At this point it is useful to compare with the *effective range expansion* for real-valued spherically symmetric potentials V obeying

$$\int_0^\infty dr\, re^{2ar} |V(r)| < \infty \qquad \text{for some} \quad a > 0. \tag{1.4.7}$$

This low-energy expansion reads (cf., e.g., [360], Ch. 12)

$$k^{2l+1} \cot \delta_l(g, k) = -[a_l(g)]^{-1} + r_l(g)k^2/2 + O(k^4),$$
$$k \geq 0, \quad g \in \mathbb{R}, \quad l = 0, 1, \ldots, \tag{1.4.8}$$

where the right-hand side of (1.4.8) is real-analytic in k^2 near $k^2 = 0$, and by definition $\delta_l(g, k)$ represent the phase shifts associated with the Schrödinger operators $-d^2/dr^2 + l(l+1)/r^2 \dotplus gV(r)$. The coefficients $a_l(g)$ and $r_l(g)$, $l = 0, 1, \ldots$, are called *partial wave scattering lengths* and *effective range parameters*, respectively. The explicit expressions

$$k \cot \boldsymbol{\delta}_{0,\alpha}(k) = 4\pi\alpha, \qquad \boldsymbol{\delta}_l(k) \equiv 0, \qquad l = 1, 2, \ldots, \tag{1.4.9}$$

for the point interaction show that the effective range expansion for this interaction is already exact in zeroth order with respect to k^2, i.e., the s-wave scattering parameters are given by

$$\begin{aligned} a_{0,\alpha} &= -(4\pi\alpha)^{-1}, \\ r_{0,\alpha} &\equiv 0 \quad \text{etc.}, \qquad -\infty < \alpha \leq \infty, \quad \alpha \neq 0, \end{aligned} \tag{1.4.10}$$

and all low-energy parameters vanish identically in higher partial waves $l = 1, 2, \ldots$. This shows in a nice way that the point interaction is in fact a zero-range interaction which acts nontrivially only in the s-wave $l = 0$. Moreover, it provides a physical interpretation of the boundary condition parameter $4\pi\alpha$ as the negative inverse scattering length.

Next let

$$\Psi_{\alpha,y}(k\omega, x) = e^{ik\omega x} + \frac{e^{ik\omega y}}{(4\pi\alpha - ik)} \frac{e^{ik|x-y|}}{|x-y|},$$

$$k \geq 0, \quad \omega \in S^2, \quad -\infty < \alpha \leq \infty, \quad x, y \in \mathbb{R}^3, \quad x \neq y. \quad (1.4.11)$$

Then obviously $\Psi_{\alpha,y}(k\omega, x)$ is the scattering wave function corresponding to $-\Delta_{\alpha,y}$ as can, e.g., be read off directly from (1.1.16), (1.4.1), and the Bessel function expansion of $e^{ik\omega(x-y)}$

$$e^{-ik\omega y}\Psi_{\alpha,y}(k\omega, x) = 4\pi|x-y|^{-1}\psi_{0,\alpha}(k|x-y|)\overline{Y_{00}(\omega)}Y_{00}(\omega_x)$$

$$+ 4\pi|x-y|^{-1} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} i^l \psi_l(k|x-y|)\overline{Y_{lm}(\omega)}Y_{lm}(\omega_x),$$

$$k \geq 0, \quad \omega \in S^2, \quad -\infty < \alpha \leq \infty, \quad x \neq y, \quad \omega_x = x/|x|. \quad (1.4.12)$$

By inspection $\Psi_{\alpha,y}(k\omega, x)$ fulfills

$$\{-4\pi\alpha|x-y|\Psi_{\alpha,y}(k\omega, x) + |x-y|^{-1}(x-y)\nabla_x\Psi_{\alpha,y}(k\omega, x)\}|_{x=y} = 0,$$

$$-(\Delta\Psi_{\alpha,y})(k\omega, x) = k^2\Psi_{\alpha,y}(k\omega, x), \qquad x \neq y, \quad (1.4.13)$$

$$\lim_{\varepsilon \downarrow 0} \lim_{\substack{|x'| \to \infty \\ -|x'|^{-1}x' = \omega}} 4\pi|x'|e^{-i(k+i\varepsilon)|x'|}[-\Delta_{\alpha,y} - (k+i\varepsilon)^2]^{-1}(x, x') = \Psi_{\alpha,y}(k\omega, x),$$

$$x \neq y; \quad k \geq 0, \quad \omega \in S^2, \quad -\infty < \alpha \leq \infty.$$

The *on-shell scattering amplitude* $f_{\alpha,y}(k, \omega, \omega')$ associated with $-\Delta_{\alpha,y}$ is then given by

$$f_{\alpha,y}(k, \omega, \omega') = \lim_{\substack{|x| \to \infty \\ |x|^{-1}x = \omega}} |x|e^{-ik|x|}[\Psi_{\alpha,y}(k\omega', x) - e^{ik\omega' x}]$$

$$= (4\pi\alpha - ik)^{-1}e^{ik(\omega' - \omega)y},$$

$$k \geq 0, \quad \omega, \omega' \in S^2, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3. \quad (1.4.14)$$

The corresponding *off-shell extension* $f_{\alpha,y}(k, p, q)$ is then defined to be

$$f_{\alpha,y}(k, p, q) = (4\pi\alpha - ik)^{-1}e^{i(p-q)y},$$

$$k \in \mathbb{C}, \quad k \neq -4\pi i\alpha, \quad p, q \in \mathbb{C}^3, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3, \quad (1.4.15)$$

and we get

$$f_{\alpha,y}(k, \omega, \omega') = f_{\alpha,y}(k, p, q)|_{|p|=|q|=k},$$

$$p, q \in \mathbb{R}^3, \quad \omega = |p|^{-1}p, \quad \omega' = |q|^{-1}q. \quad (1.4.16)$$

The unitary *on-shell scattering operator* $\mathcal{S}_{\alpha,y}(k)$ in $L^2(S^2)$ finally reads

$$\mathcal{S}_{\alpha,y}(k) = 1 - (k/2\pi i)(4\pi\alpha - ik)^{-1}(e^{-ik(\cdot)y}, \cdot)e^{-ik(\cdot)y},$$

$$k \geq 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^3, \quad (1.4.17)$$

(in particular, if we choose $y = 0$, (1.4.17) takes on the simple form $\mathcal{S}_{\alpha,0}(k) =$

$1 + 2ik(4\pi\alpha - ik)^{-1}(Y_{00}, \cdot)Y_{00})$. We also note that in the low-energy limit $k \to 0$

$$\mathscr{S}_{\alpha,y}(k) \xrightarrow[k\to 0]{n} \begin{cases} 1, & -\infty < \alpha \leq \infty, \quad \alpha \neq 0, \\ 1 - 2(Y_{00}, \cdot)Y_{00}, & \alpha = 0; \quad y \in \mathbb{R}^3, \end{cases} \tag{1.4.18}$$

and

$$-\lim_{k\to 0} f_{\alpha,y}(k, \omega, \omega') = -(4\pi\alpha)^{-1} = a_\alpha, \qquad -\infty < \alpha \leq \infty, \quad \alpha \neq 0, \quad y \in \mathbb{R}^3, \tag{1.4.19}$$

with a_α the scatterinng length obtained in (1.4.10).

As can be read off from (1.4.17), $\mathscr{S}_{\alpha,y}(k)$ has a meromorphic continuation in k to all of $\mathbb{C}$ and the pole of $\mathscr{S}_{\alpha,y}(k)$ obviously coincides with the bound state or resonance of $-\Delta_{\alpha,y}$ as long as $\alpha \neq 0$. The methods described above are entirely stationary ones. For the connection of $\mathscr{S}_{\alpha,y}$ with time-dependent scattering theory we refer to Appendix E.

Next, we briefly turn to stationary scattering theory associated with the Schrödinger operator $H_{\varepsilon,y}$. Assume V to be real-valued and

$$e^{2a|\cdot|}V \in R \qquad \text{for some} \quad a > 0 \tag{1.4.20}$$

for the rest of this section, and let u and v be as in Sect. 1.2. We introduce in $L^2(\mathbb{R}^3)$

$$\begin{aligned} &\Phi^-_{\varepsilon,y}(p, x) = u_\varepsilon(x)e^{ipx}, \\ &\Phi^+_{\varepsilon,y}(p, x) = v_\varepsilon(x)e^{ipx}; \qquad \varepsilon > 0, \quad p \in \mathbb{C}^3, \quad |\mathrm{Im}\, p| < a, \end{aligned} \tag{1.4.21}$$

where

$$u_\varepsilon(x) = u((x - y)/\varepsilon), \qquad v_\varepsilon(x) = v((x - y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3. \tag{1.4.22}$$

The *transition operator* $t_\varepsilon(k)$ then reads

$$t_\varepsilon(k) = \varepsilon^{-2}\lambda(\varepsilon)[1 + \varepsilon^{-2}\lambda(\varepsilon)u_\varepsilon G_k v_\varepsilon]^{-1},$$
$$0 < \varepsilon < \varepsilon_0, \quad \mathrm{Im}\, k > -a/\varepsilon_0, \quad k^2 \notin \mathscr{E}_\varepsilon, \tag{1.4.23}$$

where $\lambda(\cdot)$ has been introduced in Sect. 1.2 and the exceptional set $\mathscr{E}_\varepsilon$ is given by

$$\mathscr{E}_\varepsilon = \{k^2 \in \mathbb{C} | \lambda(\varepsilon)uG_{\varepsilon k}v\phi_\varepsilon = -\phi_\varepsilon \text{ for some } \phi_\varepsilon \in L^2(\mathbb{R}^3), \phi_\varepsilon \neq 0, \mathrm{Im}\, k > -a/\varepsilon_0\},$$
$$0 < \varepsilon < \varepsilon_0. \tag{1.4.24}$$

Due to condition (1.4.20), $\mathscr{E}_\varepsilon$ is discrete and a compact set of Lebesgue measure zero [434]. The *on-shell scattering amplitude* $f_{\varepsilon,y}(k, \omega, \omega')$ is then defined as

$$f_{\varepsilon,y}(k, \omega, \omega') = -(4\pi)^{-1}(\Phi^+_{\varepsilon,y}(k\omega), t_\varepsilon(k)\Phi^-_{\varepsilon,y}(k\omega')),$$
$$\varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad \omega, \omega' \in S^2, \quad y \in \mathbb{R}^3 \tag{1.4.25}$$

and its *off-shell extension* $f_{\varepsilon,y}(k, p, q)$ is given by

$$f_{\varepsilon,y}(k, p, q) = -(4\pi)^{-1}(\Phi^{+}_{\varepsilon,y}(p), t_{\varepsilon}(k)\Phi^{-}_{\varepsilon,y}(q)), \qquad 0 < \varepsilon < \varepsilon_0, \quad \operatorname{Im} k > -a/\varepsilon_0,$$
$$k^2 \notin \mathscr{E}_{\varepsilon}, \quad p, q \in \mathbb{C}^3, \quad |\operatorname{Im} p|, |\operatorname{Im} q| < a/\varepsilon_0, \quad y \in \mathbb{R}^3, \quad (1.4.26)$$

such that

$$f_{\varepsilon,y}(k, \omega, \omega') = f_{\varepsilon,y}(k, p, q)|_{|p|=|q|=k},$$
$$\varepsilon > 0, \quad y, p, q \in \mathbb{R}^3, \quad \omega = |p|^{-1}p, \quad \omega' = |q|^{-1}q. \quad (1.4.27)$$

The unitary *on-shell scattering operator* $S_{\varepsilon,y}(k)$ in $L^2(S^2)$ is defined by

$$(S_{\varepsilon,y}(k)\phi)(\omega) = \phi(\omega) - (k/2\pi i)\int_{S^2} d\omega' f_{\varepsilon,y}(k, \omega, \omega')\phi(\omega'),$$
$$\phi \in L^2(S^2), \quad \varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_{\varepsilon}, \quad \omega \in S^2, \quad y \in \mathbb{R}^3. \quad (1.4.28)$$

In order to determine the limit $\varepsilon \downarrow 0$ of $f_{\varepsilon,y}$ and $S_{\varepsilon,y}$ it essentially suffices to consider $t_{\varepsilon}(k)$ as $\varepsilon \downarrow 0$. Thus we state the following generalization of Lemma 1.2.4.

Lemma 1.4.1. *Let* $e^{2a|\cdot|}V \in R$ *for some* $a > 0$ *and* $\lambda'(0) \neq 0$ *in cases* III *and* IV. *Assume* (1.2.84) *and let* $0 < |\varepsilon| < \varepsilon_0$ *be small enough. Then* $\varepsilon[1 + B_{\varepsilon}(k)]^{-1}$, $\operatorname{Im} k > -a/\varepsilon_0$, *is analytic in* ε *near* $\varepsilon = 0$ *and the following expansion in norm holds*

$$\varepsilon[1 + B_{\varepsilon}(k)]^{-1} = \varepsilon(1 + uG_0v)^{-1} - \varepsilon^2(1 + uG_0v)^{-1}B_1(k)(1 + uG_0v)^{-1} + O(\varepsilon^3)$$
$$\textit{in case } \mathrm{I}, \quad (1.4.29)$$

$$\begin{aligned}\varepsilon[1 + B_{\varepsilon}(k)]^{-1} = {} & [(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}(\tilde{\phi}, \cdot)\phi + \varepsilon T \\ & - \varepsilon(ik/4\pi)[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}(\phi, v)(T^*v, \cdot)\phi \\ & - \varepsilon(ik/4\pi)[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}(v, \phi)(\tilde{\phi}, \cdot)Tu \\ & + \varepsilon(ik/4\pi)^2[(ik/4\pi)|(v, \phi)|^2 \\ & + \lambda'(0)]^{-2}|(v, \phi)|^2(v, Tu)(\tilde{\phi}, \cdot)\phi \\ & - \varepsilon[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-2}(\tilde{\phi}, B_2(k)\phi)(\tilde{\phi}, \cdot)\phi + O(\varepsilon^2),\end{aligned}$$
$$k \neq 0 \quad \textit{if } \lambda'(0) = 0 \quad \textit{in case } \mathrm{II}, \quad (1.4.30)$$

$$\begin{aligned}\varepsilon[1 + B_{\varepsilon}(k)]^{-1} = {} & -[\lambda'(0)]^{-1}P + \varepsilon T - \varepsilon[\lambda'(0)]^{-2}PB_2(k)P \\ & - \varepsilon^2 TB_1(k)T + \varepsilon^2[\lambda'(0)]^{-1}PB_2(k)T - \varepsilon^2[\lambda'(0)]^{-1}\cdot \\ & \cdot\{\{1 - [1 + (\lambda'(0))^{-1}]P\}[PB_2(k) + TB_1(k) - T]\}^2P \\ & + \varepsilon^2[\lambda'(0)]^{-1}\{1 - [1 + (\lambda'(0))^{-1}]P\}\cdot \\ & \cdot[PB_3(k) + TB_2(k) - T^2B_1(k)]P + O(\varepsilon^3)\end{aligned}$$
$$\textit{in case } \mathrm{III}, \quad (1.4.31)$$

$$\varepsilon[1 + B_\varepsilon(k)]^{-1} = \sum_{l,l'=1}^{N} (\tilde{\phi}, B_1(k)\phi)^{-1}_{ll'}(\tilde{\phi}_{l'}, \cdot)\phi_l + \varepsilon T$$
$$- \varepsilon(ik/4\pi)(v, \phi_1) \sum_{l=1}^{N} (\tilde{\phi}, B_1(k)\phi)^{-1}_{1l}(\tilde{\phi}_{l'}, \cdot)Tu$$
$$- \varepsilon(ik/4\pi)(\phi_1, v) \sum_{l=1}^{N} (\tilde{\phi}, B_1(k)\phi)^{-1}_{l1}(T^*v, \cdot)\phi_l$$
$$+ \varepsilon(ik/4\pi)^2(v, Tu)|(v, \phi_1)|^2 \sum_{l,l'=1}^{N} (\tilde{\phi}, B_1(k)\phi)^{-1}_{l1} \cdot$$
$$\cdot(\tilde{\phi}, B_1(k)\phi)^{-1}_{1l'}(\tilde{\phi}_{l'}, \cdot)\phi_l$$
$$- \varepsilon \sum_{l,l',l'',l'''=1}^{N} (\tilde{\phi}, B_1(k)\phi)^{-1}_{ll'}(\tilde{\phi}_{l'}, B_2(k)\phi_{l''})(\tilde{\phi}, B_1(k)\phi)^{-1}_{l''l'''} \cdot$$
$$\cdot(\tilde{\phi}_{l'''}, \cdot)\phi_l + O(\varepsilon^2)$$

in case IV. (1.4.32)

Here the analytic expansion valid in Hilbert–Schmidt norm (*cf.* (1.2.42))

$$B_\varepsilon(k) = B_0 + \sum_{n=1}^{\infty} \varepsilon^n B_n(k), \tag{1.4.33}$$

$$B_0 = uG_0v,$$
$$B_1(k) = \lambda'(0)uG_0v + (ik/4\pi)(v, \cdot)u, \tag{1.4.34}$$
$$B_2(k) = [\lambda''(0)/2]uG_0v + (ik/4\pi)\lambda'(0)(v, \cdot)u + k^2C,$$

(*C defined in* (1.3.6)), *etc., has been used. In case* IV

$$(\tilde{\phi}, B_1(k)\phi)^{-1}_{ll'} = [(ik/4\pi)|(v, \phi_1)|^2\delta_{l1}\delta_{l'1} + \lambda'(0)]^{-1}\delta_{ll'} \tag{1.4.35}$$

denotes the inverse of the matrix $(\tilde{\phi}_l, B_1(k)\phi_{l'})$, $l, l' = 1, \ldots, N$.

PROOF. *Case* I: Since $(1 + uG_0v)^{-1}$ exists, (1.4.29) immediately results by inserting expansion (1.4.33) for $B_\varepsilon(k)$ into $[1 + B_\varepsilon(k)]^{-1}$.

Case II: We partly follow the proof of Theorem 1.3.1(b) and expand (cf. (1.3.17))

$$\varepsilon[1 + B_\varepsilon(k)]^{-1} = \varepsilon\{1 - [1 + B_\varepsilon(k) + P]^{-1}P\}^{-1}[1 + B_\varepsilon(k) + P]^{-1}$$
$$= \varepsilon\{1 - P + \varepsilon[P + T][B_1(k) + O(\varepsilon)]P\}^{-1}[P + T + O(\varepsilon)],$$
$$|\varepsilon| \text{ small enough.} \tag{1.4.36}$$

Formula (1.3.47) then shows that $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ is analytic in ε near $\varepsilon = 0$ since after identifying $\mathscr{H} = L^2(\mathbb{R}^3)$, $\beta = 1$, $\tilde{\psi} = \tilde{\phi}$, $\psi = \phi$, $R = \varepsilon[P + T]B_1(k)P$ one infers that

$$\varepsilon\{1 + (\tilde{\phi}, \{1 + \varepsilon[P + T]B_1(k)P\}^{-1}\phi)\}^{-1} = -[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1} + O(\varepsilon) \tag{1.4.37}$$

is analytic in ε near $\varepsilon = 0$. The right-hand side of (1.4.30) then results after an explicit expansion of (1.4.36) in terms of ε.

Case III: We again expand as in (1.4.36). Since now P is, in general, of rank N we use the formula (cf. Lemma B.5)

$$\left[1 + \beta \sum_{l=1}^{N} (\tilde{\psi}_l, \cdot)\psi_l + R\right]^{-1} = [1 + R]^{-1} - \beta \sum_{l,l'=1}^{N} \{1 + \beta(\tilde{\psi}, [1 + R]^{-1}\psi)\}_{ll'}^{-1} \cdot$$
$$\cdot([1 + R^*]^{-1}\tilde{\psi}_{l'}, \cdot)[1 + R]^{-1}\psi_l, \tag{1.4.38}$$

where $\beta \in \mathbb{C}$, $\tilde{\psi}_l, \psi_l \in \mathscr{H}$, R, $[1 + R]^{-1} \in \mathscr{B}(\mathscr{H})$ for some separable Hilbert space $\mathscr{H}$ and the existence of the inverse matrix of $\{\delta_{ll'} + \beta(\tilde{\psi}_l, [1 + R]^{-1}\psi_{l'})\}$ denoted by $\{1 + \beta(\tilde{\psi}, [1 + R]^{-1}\psi)\}_{ll'}^{-1}$, $l, l' = 1, \ldots, N$, is assumed. Using $Pu = 0$ and identifying $\beta = 1$, $\tilde{\psi}_l = \tilde{\phi}_l$, $\psi_{l'} = \phi_{l'}$, $R = \varepsilon[P + T]B_1(k)P = -\varepsilon\lambda'(0)P$ we again infer that $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ is analytic in ε near $\varepsilon = 0$ since

$$\varepsilon\{1 + (\tilde{\phi}, [1 - \varepsilon\lambda'(0)P]^{-1}\phi)\}_{ll'}^{-1} = [\lambda'(0)]^{-1}\delta_{ll'} + O(\varepsilon) \tag{1.4.39}$$

is analytic in ε near $\varepsilon = 0$. The expansion coefficients on the right-hand side of (1.4.31) now follow by a straightforward calculation.

Case IV: The proof is identical to that of case III up to the point that now, similar to case II, $R = \varepsilon[P + T]B_1(k)P$ has to be used. Analyticity of $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ in ε near $\varepsilon = 0$ now follows from that of

$$\varepsilon\{1 + (\tilde{\phi}, [1 + \varepsilon(P + T)B_1(k)P]^{-1}\phi)\}_{ll'}^{-1}$$
$$= -[(ik/4\pi)|(v, \phi_1)|^2\delta_{l1}\delta_{l'1} + \lambda'(0)]^{-1}\delta_{ll'} + O(\varepsilon). \tag{1.4.40}$$

∎

Given Lemma 1.4.1 we are able to expand the off-shell scattering amplitude $f_{\varepsilon,y}(k, p, q)$ with respect to ε near $\varepsilon = 0$:

Theorem 1.4.2. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued and assume $\lambda'(0) \neq 0$ in cases* III *and* IV. *Assume* (1.2.84) *and let $|\varepsilon| < \varepsilon_0$ be small enough. Then $f_{\varepsilon,y}(k, p, q)$, $\mathrm{Im}\, k > -a/\varepsilon_0$, $|\mathrm{Im}\, p|$, $|\mathrm{Im}\, q| < a/\varepsilon_0$, $y \in \mathbb{R}^3$, is analytic in ε near $\varepsilon = 0$ and*

$$\begin{aligned} -4\pi e^{iy(p-q)}f_{\varepsilon,y}(k, p, q) = {} & \varepsilon(v, (1 + uG_0v)^{-1}u) - \varepsilon^2(ik/4\pi)(v, (1 + uG_0v)^{-1}u)^2 \\ & + \varepsilon^2\lambda'(0)(v, (1 + uG_0v)^{-2}u) \\ & - i\varepsilon^2(p(\cdot)v, (1 + uG_0v)^{-1}u) \\ & + i\varepsilon^2((1 + vG_0u)^{-1}v, q(\cdot)u) + O(\varepsilon^3) \end{aligned}$$
$$\textit{in case } \mathrm{I}, \tag{1.4.41}$$

$$\begin{aligned} -4\pi e^{iy(p-q)}f_{\varepsilon,y}(k, p, q) = {} & -4\pi e^{iy(p-q)}f_{\alpha,y}(k, p, q) \\ & + \varepsilon\lambda'(0)[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1}|(v, \phi)|^2 \\ & + \varepsilon[\lambda'(0)]^2[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-2} \cdot \\ & \cdot (v, (1 + uG_0v)^{-1}u) - \varepsilon[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-2} \cdot \\ & \cdot |(v, \phi)|^2(\tilde{\phi}, B_2(k)\phi) - i\varepsilon[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1} \cdot \\ & \cdot (\phi, v)(p(\cdot)v, \phi) + i\varepsilon[(ik/4\pi)|(v, \phi)|^2 + \lambda'(0)]^{-1} \cdot \\ & \cdot (v, \phi)(\phi, q(\cdot)v) + O(\varepsilon^2), \end{aligned}$$

$$\alpha = -\lambda'(0)|(v, \phi)|^{-2}, \quad k \neq 0 \quad \textit{if } \lambda'(0) = 0 \quad \textit{in case } \mathrm{II}, \tag{1.4.42}$$

$$-4\pi e^{iy(p-q)} f_{\varepsilon,y}(k,p,q) = \varepsilon(v, Tu) - \varepsilon^2(ik/4\pi)(v, Tu)^2 + \varepsilon^2\lambda'(0)(v, T^2u)$$
$$+ \varepsilon^2[\lambda'(0)]^{-1}\sum_{l=1}^{N}(p(\cdot)v, \phi_l)(\phi_l, q(\cdot)v)$$
$$- i\varepsilon^2(p(\cdot)v, Tu) + i\varepsilon^2(T^*v, q(\cdot)u) + O(\varepsilon^3)$$
$$\textit{in case III}, \quad (1.4.43)$$

$$-4\pi e^{iy(p-q)} f_{\varepsilon,y}(k,p,q) = -4\pi e^{iy(p-q)} f_{\alpha,y}(k,p,q)$$
$$+ \varepsilon\lambda'(0)[(ik/4\pi)|(v,\phi_1)|^2 + \lambda'(0)]^{-1}|(v,\phi_1)|^2$$
$$+ \varepsilon[\lambda'(0)]^2[(ik/4\pi)|(v,\phi_1)|^2 + \lambda'(0)]^{-2}(v, Tu)$$
$$- \varepsilon|(\phi_1, v)|^2 \sum_{l,l'=1}^{N}(\tilde{\phi}, B_1(k)\phi)^{-1}_{1l}(\tilde{\phi}_l, B_2(k)\phi_{l'})\cdot$$
$$\cdot(\tilde{\phi}, B_1(k)\phi)^{-1}_{l'1}$$
$$- i\varepsilon(\phi_1, v)\sum_{l=1}^{N}(p(\cdot)v, \phi_l)(\tilde{\phi}, B_1(k)\phi)^{-1}_{l1}$$
$$+ i\varepsilon(v, \phi_1)\sum_{l=1}^{N}(\tilde{\phi}, B_1(k)\phi)^{-1}_{1l}(\phi_l, q(\cdot)v) + 0(\varepsilon^2),$$
$$\alpha = -\lambda'(0)|(v,\phi_1)|^{-2} \quad \textit{in case IV}. \quad (1.4.44)$$

PROOF. By a translation $x \to x + y$ and a scaling transformation $x \to \varepsilon x$ using (1.2.15) we obtain

$$f_{\varepsilon,y}(k,p,q) = -(4\pi)^{-1}e^{-iy(p-q)}\lambda(\varepsilon)(ue^{i\varepsilon px}, \varepsilon[1 + B_\varepsilon(k)]^{-1}ve^{i\varepsilon qx'}), \quad (1.4.45)$$

where in obvious notation $x, x' \in \mathbb{R}^3$ denote integration variables. The above results now directly follow by inserting Lemma 1.4.1 into (1.4.45) and expanding $\lambda(\varepsilon)$, $e^{i\varepsilon px}$, $e^{i\varepsilon qx'}$ with respect to ε. ■

It remains to derive the corresponding expansion for $S_{\varepsilon,y}(k)$ near $\varepsilon = 0$:

Theorem 1.4.3. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued, $\lambda'(0) \neq 0$ in cases* III *and* IV *and assume (1.2.84). Then $S_{\varepsilon,y}(k)$, $k \geq 0$, $y \in \mathbb{R}^3$, is analytic in ε near $\varepsilon = 0$ and for $|\varepsilon|$ small enough we get*

$$S_{\varepsilon,y}(k) = 1 + (2\pi i)^{-1}\varepsilon k(v, (1 + uG_0v)^{-1}u)(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00}$$
$$- (8\pi^2)^{-1}(\varepsilon k)^2(v, (1 + uG_0v)^{-1}u)^2(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00}$$
$$+ (2\pi i)^{-1}\varepsilon^2 k\lambda'(0)(v, (1 + uG_0v)^{-2}u)(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00}$$
$$- (\varepsilon k)^2(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_1 + (\varepsilon k)^2(e^{-ik(\cdot)y}Y_1, \cdot)e^{-ik(\cdot)y}Y_{00}$$
$$+ O(\varepsilon^3) \quad \textit{in case I}, \quad (1.4.46)$$

where

$$Y_1(\omega) = (4\pi^{3/2})^{-1}\int_{\mathbb{R}^3} d^3x\, \omega x v(x)((1 + uG_0v)^{-1}u)(x), \qquad \omega \in S^2. \quad (1.4.47)$$

$$
\begin{aligned}
S_{\varepsilon,y}(k) = {} & \mathscr{S}_{\alpha,y}(k) + (2\pi i)^{-1}\varepsilon k\lambda'(0)[(ik/4\pi)|(v,\phi)|^2 + \lambda'(0)]^{-1}\cdot \\
& \cdot|(v,\phi)|^2(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& + (2\pi i)^{-1}\varepsilon k[\lambda'(0)]^2[(ik/4\pi)|(v,\phi)|^2 + \lambda'(0)]^{-2}(v,(1+uG_0v)^{-1}u)\cdot \\
& \cdot(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& - (2\pi i)^{-1}\varepsilon k[(ik/4\pi)|(v,\phi)|^2 + \lambda'(0)]^{-2}|(v,\phi)|^2(\tilde{\phi},B_2(k)\phi)\cdot \\
& \cdot(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} - \varepsilon k^2[(ik/4\pi)|(v,\phi)|^2 + \lambda'(0)]^{-1}\cdot \\
& \cdot(\phi,v)(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}\hat{Y}_1 + \varepsilon k^2[(ik/4\pi)|(v,\phi)|^2 + \lambda'(0)]^{-1}\cdot \\
& \cdot(v,\phi)(e^{-ik(\cdot)y}\hat{Y}_1,\cdot)e^{-ik(\cdot)y}Y_{00} + O(\varepsilon^2), \\
& \alpha = -\lambda'(0)|(v,\phi)|^{-2}, \quad k \neq 0 \quad \textit{if } \lambda'(0) = 0 \quad \textit{in case } \mathrm{II}, \qquad (1.4.48)
\end{aligned}
$$

where

$$\hat{Y}_1(\omega) = (4\pi^{3/2})^{-1}\int_{\mathbb{R}^3} d^3x\,\omega x v(x)\phi(x), \qquad \omega \in S^2. \tag{1.4.49}$$

$$
\begin{aligned}
S_{\varepsilon,y}(k) = {} & 1 + (2\pi i)^{-1}\varepsilon k(v,Tu)(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& - (8\pi^2)^{-1}(\varepsilon k)^2(v,Tu)^2(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& + (2\pi i)^{-1}\varepsilon^2 k\lambda'(0)(v,T^2u)(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& + 2\pi\varepsilon^2 k^3[\lambda'(0)]^{-1}\sum_{l=1}^{N}(e^{-ik(\cdot)y}\hat{Y}_{1,l},\cdot)e^{-ik(\cdot)y}\hat{Y}_{1,l} \\
& - (\varepsilon k)^2(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}\tilde{Y}_1 \\
& + (\varepsilon k)^2(e^{-ik(\cdot)y}\tilde{Y}_1,\cdot)e^{-ik(\cdot)y}Y_{00} + O(\varepsilon^3) \quad \textit{in case } \mathrm{III}, \qquad (1.4.50)
\end{aligned}
$$

where

$$\tilde{Y}_1(\omega) = (4\pi^{3/2})^{-1}\int_{\mathbb{R}^3} d^3x\,\omega x v(x)(Tu)(x), \qquad \omega \in S^2. \tag{1.4.51}$$

$$
\begin{aligned}
S_{\varepsilon,y}(k) = {} & \mathscr{S}_{\alpha,y}(k) + (2\pi i)^{-1}\varepsilon k\lambda'(0)[(ik/4\pi)|(v,\phi_1)|^2 + \lambda'(0)]^{-1}|(v,\phi_1)|^2\cdot \\
& \cdot(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& + (2\pi i)^{-1}\varepsilon k[\lambda'(0)]^2[(ik/4\pi)|(v,\phi_1)|^2 + \lambda'(0)]^{-2}(v,Tu)\cdot \\
& \cdot(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& - (2\pi i)^{-1}\varepsilon k|(v,\phi_1)|^2\sum_{l,l'=1}^{N}(\tilde{\phi},B_1(k)\phi)^{-1}_{1l}(\tilde{\phi}_l,B_2(k)\phi_{l'})(\tilde{\phi},B_1(k)\phi)_{l'1}\cdot \\
& \cdot(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}Y_{00} \\
& - \varepsilon k^2(\phi_1,v)\sum_{l=1}^{N}(\tilde{\phi},B_1(k)\phi)^{-1}_{l1}(e^{-ik(\cdot)y}Y_{00},\cdot)e^{-ik(\cdot)y}\hat{Y}_{1,l} \\
& + \varepsilon k^2(v,\phi_1)\sum_{l=1}^{N}(\tilde{\phi},B_1(k)\phi)^{-1}_{1l}(e^{-ik(\cdot)y}\hat{Y}_{1,l},\cdot)e^{-ik(\cdot)y}Y_{00} + O(\varepsilon^2), \\
& \alpha = -\lambda'(0)|(v,\phi_1)|^{-2} \quad \textit{in case } \mathrm{IV}, \qquad (1.4.52)
\end{aligned}
$$

where

$$\hat{Y}_{1,l}(\omega) = (4\pi^{3/2})^{-1} \int_{\mathbb{R}^3} d^3x\, \omega x v(x)\phi_l(x), \qquad \omega \in S^2. \qquad (1.4.53)$$

PROOF. Theorem 1.4.3 is an immediate consequence of (1.4.28) and Theorem 1.4.2. ∎

Finally, we would like to add some comments concerning the above results. First of all, the expansion coefficients in Theorem 1.4.3 have been written in such a way that the results are particularly simple for $y = 0$. Next, we emphasize that only in cases II and IV (i.e., if $H = -\Delta \dotplus V$ has a zero-energy resonance) the limits of $f_{\varepsilon,y}$ and $S_{\varepsilon,y}$ as $\varepsilon \to 0$ are nontrivial and coincide with $f_{\alpha,y}$ and $\mathscr{S}_{\alpha,y}$ with α given by (1.2.53). The coefficients $(4\pi)^{-1}(v, (1 + uG_0v)^{-1}u)$ and $(4\pi)^{-1}(v, Tu)$ in $f_{\varepsilon,y}$ in cases I and III just represent the scattering length of $H = -\Delta \dotplus V$ [11]. In the special case where V is spherically symmetric (cf. the discussion before Lemma 1.2.4) we have $Y_1 = \tilde{Y}_1 = 0$ and $\hat{Y}_1$, $\hat{Y}_{1,l}$ are nonzero only if ϕ (resp. ϕ_l, $l = 1, \ldots, N$) have angular momentum one (i.e., p-waves). The expansions in Theorems 1.4.2 and 1.4.3 clearly illustrate the fact that scattering near threshold is largely independent of the detailed shape of the interaction.

As in Sects. 1.1 and 1.2 the above results immediately extend to complex point interactions with $\operatorname{Im} \alpha < 0$. In this case $\mathscr{S}_{\alpha,y}(k)$ and $S_{\varepsilon,y}(k)$ become contractions in $L^2(S^2)$.

Notes

Section I.1.1

The one-center point interaction Hamiltonian in three dimensions seems first to have been studied by Bethe and Peierls in 1935 [86] in the study of the "diplon," i.e., the system consisting of a proton and a neutron. (Wigner [497] had shown that the interaction between a proton and a neutron is of very short-range which makes it reasonable to try to define a zero-range interaction, i.e., a delta potential.) The manner in which they treat this singular interaction resembles in some way the rigorous study we have given here. First, they argue that it is only necessary to study s-waves, i.e., the subspace corresponding to $l = 0$ in (1.1.9) because "the centrifugal force makes the wave function very small for distances small compared with the wave length and the potential at still small distances will not matter." By physical arguments they deduce that the logarithmic derivative at zero of the radius times the wave function should be a constant which is directly related to the energy. Inspecting the boundary condition (1.1.12) which we imposed for s-waves we see that it is indeed equivalent to

$$\frac{d}{dr}(\ln(r\Psi))|_{r=0+} = 4\pi\alpha,$$

where $\phi(r) = r\Psi(r) \in \mathscr{D}(h_{0,\alpha})$. Thomas [485], also studying the neutron–proton system, gave in addition the form $V(r) \approx \varepsilon^{-2} f(r/\varepsilon)$ with $\varepsilon \approx 0$ for the point interaction. This point of view is studied in detail in Sect. I.1.2.

Fermi, in 1936, used a similar procedure as Bethe and Peierls when he studied the motion of neutrons in hydrogenous substances [179]. Indirectly, he proposed to replace $\delta(r)$ by

$$-\alpha^{-1}\delta(r)\frac{\partial}{\partial r} r\bigg|_{r=0+},$$

what has later been called the Fermi pseudopotential and was made more explicit by Breit in 1947 [110]. The reasoning they used was essentially the following (see [93]): The Schrödinger equation for the proton–neutron system with the center of mass motion removed is

$$H_\alpha \Psi = -\Delta\Psi = E\Psi,$$

where $\Psi = \Psi(x, y, z)$ and (x, y, z) are the relative coordinates. The interaction is given by the boundary condition above. Integrating the boundary condition yields

$$\ln(r\Psi) = 4\pi\alpha r$$

or

$$\Psi = \frac{e^{4\pi\alpha r}}{r} = \frac{1 + 4\pi\alpha r + \frac{1}{2}(4\pi\alpha r)^2 + \cdots}{r} = \left[1 + \frac{(4\pi\alpha)^{-1}}{r}\right]\phi,$$

where ϕ is regular at $r = 0$ (i.e., $\phi(0+)$ is finite). This yields for small r

$$r^2\frac{\partial\Psi}{\partial r} \approx -(4\pi\alpha)^{-1}\frac{\partial(r\Psi)}{\partial r}.$$

Integrating this over the surface of a small sphere we obtain that the left-hand side is equal to

$$\int r^2\, d\Omega\,\frac{\partial\Psi}{\partial r} = \int dS\, \nabla\Psi\cdot n = \int dV\,\Delta\Psi$$

and the right-hand side equals

$$-(4\pi\alpha)^{-1}\int d\Omega\,\frac{\partial(r\Psi)}{\partial r} = -\alpha^{-1}\phi\int dV\,\delta(r),$$

where we used

$$\frac{\partial(r\Psi)}{\partial r} \approx \phi$$

for r small enough. This implies that the integrands of the right- and left-hand sides are equal in the limit when r tends to zero, i.e.,

$$\Delta\Psi = -\alpha^{-1}\delta(r)\frac{\partial(r\Psi)}{\partial r}\bigg|_{r=0+},$$

which is small except near the origin while H_α is small near the origin. Adding the two expressions for $\Delta\Psi$ we finally obtain

$$H_\alpha \Psi = -\Delta\Psi - \alpha^{-1}\delta(r)\frac{\partial}{\partial r} r\Psi\bigg|_{r=0+} = E\Psi.$$

For recent treatments of the Fermi pseudopotential see [62], [229], [427], [428], [472], [490]. Following Grossmann and Wu [229] we can use the above heuristic formula for H_α to obtain its Green's function. The Green's function $G_{\alpha,k}$ satisfies

$$(-\Delta - k^2)G_{\alpha,k}(x, x') - \alpha^{-1}\delta(x)\frac{\partial}{\partial |x|}|x|\, G_{\alpha,k}(x, x')\bigg|_{|x|=0} = \delta(x - x').$$

Hence

$$(-\Delta - k^2)G_{\alpha,k}(x, x') = \delta(x - x') + A_\alpha(x')\delta(x),$$

where

$$A_\alpha(x') = \alpha^{-1}\frac{\partial}{\partial |x|}|x|\, G_{\alpha,k}(x, x')\bigg|_{x=0}.$$

This implies

$$G_{\alpha,k}(x, x') = G_k(x - x') + A_\alpha(x')G_k(x),$$

where G_k is the free Green's function, i.e.,

$$G_k(x) = \frac{e^{ik|x|}}{4\pi|x|}.$$

A_α is now determined by inserting the expression for $G_{\alpha,k}$ into the definition of A_α, and we find (cf. (1.1.21))

$$G_{\alpha,k}(x, x') = G_k(x - x') + \left(\alpha - \frac{ik}{4\pi}\right)^{-1} G_k(x)G_k(x').$$

Other studies of δ-interactions appeared in [277], where the N-center problem is also treated, and in [464], [509]. An extensive study of applications to atomic physics appeared in the monograph by Demkov and Ostrovskii [151]. Applications to hadron spectroscopy can be found in [87].

The rigorous study of point interactions was started in the early 1960s by Berezin and Faddeev [81] in an attempt to study the three-body problem rigorously. This work is reviewed in [184]. Berezin and Faddeev use both the method of self-adjoint extensions of symmetric operators and a method which uses a renormalization of the coupling constant in front of the δ-function. We will return to this technique in the N-center case, Ch. 1 of Part II.

The method using Dirichlet forms was introduced by Albeverio, Høegh-Krohn, and Streit [32], [33] (cf. Appendix F for an extensive discussion).

Methods of nonstandard analysis were started by Nelson [355] using (standard) results by Friedman [187], [188] who showed how to obtain point interactions as strong resolvent limits of Schrödinger operators with characteristic functions of decreasing support as the potential. This was subsequently generalized by Alonso [37] and Albeverio, Fenstad, and Høegh-Krohn [12] where the N-center case is also studied using nonstandard analysis. See also [14] and Appendix H.

As the last method to define the point interaction Hamiltonian rigorously we mention that we can simply start with the resolvent (1.1.18) and show that this is the resolvent of a self-adjoint operator. This point of view was advocated by Grossmann, Høegh-Krohn, and Mebkhout [226] using scales of Hilbert spaces (cf. Appendix G). Complex point interactions were studied in [226] and [114]. Generalized pointlike interactions appeared in [369], [370], [400b], [427], [428], [430], [431], [446].

More general systems of the type $-\Delta + V +$ "$\lambda\delta$" are discussed in [167], [171], [209], [211], [269], [416], [420], [512].

Electric and magnetic fields in connection with $-\Delta_{\alpha,y}$ are studied in [147], [148], [472].

Section I.1.2

In the special case of a square well potential V strong resolvent convergence of H_ε to $-\Delta_{\alpha,y}$ (resp. to $-\Delta$) has been discussed by Friedman [187], [188] (cf. also [37], [355]). The general local case where $V \in R$ and $(1 + |\cdot|)V \in L^1(\mathbb{R}^3)$ is due to Albeverio and Høegh-Krohn [24]. Theorem 1.2.5 is a slightly improved version of corresponding results in [16], [17] and [22] which yield norm resolvent convergence of H_ε to $-\Delta_{\alpha,y}$ (strong resolvent convergence if $\lambda'(0) = 0$ in cases III and IV is also discussed in [17]). For previous discussions of Lemma 1.2.3 and of cases I–IV under different hypotheses on V we refer to [272], [298], [357], [504]. Strong resolvent convergence in the context of Dirichlet forms has been obtained in [33], [35].

Special approximations by means of separable interactions appeared in [81], [112], [129], [512]. A detailed treatment of nonlocal interactions can be found in [98] (cf. also [200], [358]). Theorem 1.2.10 appears to be new.

Various approximation results in connection with more general systems of the type $-\Delta + V +$ "$\lambda\delta$" can be found in [171], [414], [416], [420].

Section I.1.3

Most of the results of this section are new (some of them have been announced in [17]). Our definition of resonances of $H = -\Delta \dot{+} V$, $e^{2a|\cdot|}V \in R$ for some $a > 0$, as poles of $(1 + uG_k v)^{-1}$ in the strip $0 > \operatorname{Im} k > -a$ follows the treatment in [21], [26], [28] and [200] (these papers also contain an extensive list of references on this subject). For references on perturbation theory of resonances using similar techniques see [385], [386]. Since, by relation (1.2.11), every bound state k_ε of $H_{\varepsilon,y}$ corresponds to a bound state $k(\varepsilon) = \varepsilon k_\varepsilon$ of $H(\varepsilon) = -\Delta \dot{+} \lambda(\varepsilon)V$ and vice versa, we recover the results of [298] concerning the absorption of negative bound states into the continuous spectrum at so-called critical potential strengths. In fact, Theorem 1.3.1 extends their three-dimensional results insofar as our Fredholm determinant approach allows us to calculate the leading order coefficients explicitly (it suffices to take $\lambda(\varepsilon) = 1 + \varepsilon\lambda'(0)$, $\lambda'(0) \neq 0$ and to replace all $k_{l,\varepsilon}$ in Theorem 1.3.1(b)–(d) by $\varepsilon k_{l,\varepsilon}$, $l = 1, \ldots, N$). Theorem 1.3.2 finally extends the whole treatment to resonances of $H(\varepsilon)$ by using the same type of substitution $k_\varepsilon \to k(\varepsilon) = \varepsilon k_\varepsilon$. A unified treatment of bound states and resonances of $H(\varepsilon)$ along these lines appeared in [204].

The whole discussion of this section extends to nonlocal interactions in a straightforward manner. The only changes needed in Theorem 1.3.1 are the following:

$$e^{2a|\cdot|}V \in R \to e^{a|\cdot|}\tilde{\tilde{u}}_1, e^{a|\cdot|}\tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3) \quad \text{for some } a > 0,$$

$$(v, \phi) \to (v_1, \phi) \quad \text{in case II,}$$

$$(v, \phi_1) \to (v_1, \phi_1) \quad \text{in case IV,}$$

$$C(x, x') = -(8\pi)^{-1}u(x)|x - x'|v(x')$$

$$\to C(x, x') = -(8\pi)^{-1} \int_{\mathbb{R}^6} d^3x''\, d^3x''' \cdot$$

$$\cdot W_2(x, x'')|x'' - x'''|\, W_1(x''', x').$$

In Theorem 1.3.2 one simply replaces $e^{2a|\cdot|}V \in R$ for all $a > 0$ by $e^{a|\cdot|}\tilde{\tilde{u}}_1$, $e^{a|\cdot|}\tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ for all $a > 0$ in addition to the last three substitutions stated above.

Section I.1.4

Scattering theory for point interactions from various points of view have been studied in [81], [87], [114], [184], [200], [252], [277], [369], [370], [483], [509], [512]. Stationary scattering theory for Schrödinger operators of the type $H = -\Delta \dotplus V$, $e^{2a|\cdot|}V \in R$ for some $a > 0$ can be found in [434], Ch. V, [390], Ch. XI.6. For the general formalism of scattering theory we also refer to [39], [360], [480]. Low-energy scattering for three-dimensional systems has been discussed in [16], [17], [272], [357], [358] (see also [351]). A systematic way of calculating the expansion coefficients for the transition operator $t(k)$, as $k \to 0$ by the use of recursion relations, has been developed in [101].

Low-energy parameters in connection with a detailed investigation of scattering near threshold appeared in [11]. Theorem 4.1 is taken from [17] where a slightly different proof can be found. In particular, this paper also contains a complete discussion of the case $\lambda'(0) = 0$ in cases III and IV without the simplifying assumption (1.2.84).

If one is interested in asymptotic expansions for $f_\varepsilon(k, \omega, \omega')$ and $S_{\varepsilon,y}(k)$ near $\varepsilon = 0$ instead of analytic expansions, the assumptions on V can be drastically reduced. In fact, as long as $\mathscr{E}_\varepsilon \cap (0, \varepsilon_0) = \varnothing$ for all $0 < \varepsilon < \varepsilon_0$, the conditions $V \in R$, $(1 + |x|^m)V \in L^1(\mathbb{R}^3)$ for suitable $m \in \mathbb{N}$ yield asymptotic expansions in Theorems 1.4.2 and 1.4.3, the order of which depends on m.

Again Lemma 1.4.1–Theorem 1.4.3 extend to nonlocal interactions (cf. [98]

for a detailed treatment of low-energy parameters and scattering near threshold). Here it suffices to note that the on-shell scattering amplitude associated with (1.2.65) reads

$$f_{\varepsilon,y}(k,\omega,\omega') = -(4\pi)^{-1}(\Phi^{+}_{\varepsilon,y}(k\varepsilon), t_\varepsilon(k)\Phi^{-}_{\varepsilon,y}(k\omega')),$$
$$\varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad \omega, \omega' \in S^2, \quad y \in \mathbb{R}^3$$

where now

$$\Phi^{-}_{\varepsilon,y}(p,x) = \int_{\mathbb{R}^3} d^3x'\, W_{2,\varepsilon}(x,x')e^{ipx'},$$

$$\Phi^{+}_{\varepsilon,y}(p,x) = \int_{\mathbb{R}^3} d^3x'\, \overline{W_{1,\varepsilon}(x',x)}e^{ipx'}, \qquad \varepsilon > 0, \quad p \in \mathbb{C}^3, \quad |\mathrm{Im}\, p| < a,$$

$$t_\varepsilon(k) = \varepsilon^{-2}\lambda(\varepsilon)[1 + \varepsilon^{-2}\lambda(\varepsilon)W_{2,\varepsilon}G_k W_{1,\varepsilon}]^{-1},$$
$$0 < \varepsilon < \varepsilon_0, \quad \mathrm{Im}\, k > -a/\varepsilon_0, \quad k^2 \notin \mathscr{E}_\varepsilon,$$

$$\mathscr{E}_\varepsilon = \{k^2 \in \mathbb{C} \,|\, \lambda(\varepsilon)W_2 G_{\varepsilon k} W_1 \phi_\varepsilon = -\phi_\varepsilon \text{ for some } \phi_\varepsilon \in L^2(\mathbb{R}^3),$$
$$\phi_\varepsilon \neq 0, \mathrm{Im}\, k > -a/\varepsilon_0\}, \qquad 0 < \varepsilon < \varepsilon_0,$$

$$W_{j,\varepsilon}(x,x') = \varepsilon^{-3}W_j(\varepsilon^{-1}(x-y), \varepsilon^{-1}(x'-y)), \qquad \varepsilon > 0, \quad j = 1, 2, \quad y \in \mathbb{R}^3$$

using the assumption $e^{a|\cdot|}\tilde{\tilde{u}}_1, e^{a|\cdot|}\tilde{\tilde{v}}_2 \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ for some $a > 0$.

CHAPTER I.2

Coulomb Plus One-Center Point Interaction in Three Dimensions

I.2.1 Basic Properties

In this section we extend the analysis of Sect. 1.1 to include the Coulomb potential in addition to the point interaction both centered at a fixed point $y \in \mathbb{R}^3$. Following very closely the approach in Sect. 1.1 we again concentrate on the methods of self-adjoint operator extensions.

In the Hilbert space $L^2(\mathbb{R}^3)$ we consider the operator

$$(-\Delta + \gamma|\cdot - y|^{-1})|_{C_0^\infty(\mathbb{R}^3 - \{y\})}, \qquad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \tag{2.1.1}$$

and denote by $\dot{H}_{\gamma,y}$ its closure in $L^2(\mathbb{R}^3)$ (i.e., $\mathscr{D}(\dot{H}_{\gamma,y}) = H_0^{2,2}(\mathbb{R}^3 - \{y\})$). Then its adjoint is given by [274], [276]

$$(\dot{H}_{\gamma,y})^* = -\Delta + \gamma|\cdot - y|^{-1},$$

$$\mathscr{D}((\dot{H}_{\gamma,y})^*) = \{g \in H_{\text{loc}}^{2,2}(\mathbb{R}^3 - \{y\}) \cap L^2(\mathbb{R}^3) | (-\Delta g + \gamma|\cdot - y|^{-1} g) \in L^2(\mathbb{R}^3)\},$$

$$y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \tag{2.1.2}$$

By inspection, one infers that

$$\psi_\gamma(k, x) = |x - y|^{-1} \mathscr{W}_{-i\gamma/2k;\, 1/2}(-2ik|x - y|),$$

$$\operatorname{Im} k > 0, \quad \gamma \in \mathbb{R}, \quad x \in \mathbb{R}^3 - \{y\}, \tag{2.1.3}$$

where $\mathscr{W}_{\mu;\nu}(\cdot)$ denotes the Whittaker function [1], is the unique solution of

$$(\dot{H}_{\gamma,y})^* \psi(k) = k^2 \psi(k), \quad \psi(k) \in \mathscr{D}((\dot{H}_{\gamma,y})^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0. \tag{2.1.4}$$

Thus $\dot{H}_{\gamma,y}$ has deficiency indices (1, 1) and applying Theorem A.1 all self-adjoint extensions $H_{\gamma,\theta,y}$ of $\dot{H}_{\gamma,y}$ are given by the one-parameter family

$$\mathscr{D}(H_{\gamma,\theta,y}) = \{g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-} | g \in \mathscr{D}(\dot{H}_{\gamma,y}),\ a \in \mathbb{C}\},$$

$$H_{\gamma,\theta,y}(g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-}) = \dot{H}_{\gamma,y}g + ia\psi_{\gamma+} - iae^{i\theta}\psi_{\gamma-}, \tag{2.1.5}$$
$$\theta \in [0, 2\pi), \quad y \in \mathbb{R}^3,$$

where

$$\psi_{\gamma\pm}(x) = |x - y|\,\mathscr{W}_{-i\gamma/2(\pm i)^{1/2};\,1/2}(-2i(\pm i)^{1/2}|x - y|),$$
$$\operatorname{Im}(\pm i)^{1/2} > 0, \quad \gamma \in \mathbb{R}, \quad x \in \mathbb{R}^3 - \{y\}. \tag{2.1.6}$$

Next, we introduce spherical coordinates like those in Sect. 1.1 since $\dot{H}_{\gamma,y}$ is obviously spherically symmetric around $y \in \mathbb{R}^3$. With respect to the decomposition (1.1.9), $\dot{H}_{\gamma,y}$ then equals the direct sum

$$\dot{H}_{\gamma,y} = T_y^{-1}\left\{\bigoplus_{l=0}^{\infty} U^{-1}\dot{h}_{\gamma,l}U \otimes 1\right\}T_y, \qquad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \tag{2.1.7}$$

where T_y implements translations $x \to x + y$ in $L^2(\mathbb{R}^3)$, $(T_y g)(x) = g(x + y)$, $g \in L^2(\mathbb{R}^3)$, $y \in \mathbb{R}^3$, and

$$\dot{h}_{\gamma,l} = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{\gamma}{r}, \qquad \gamma \in \mathbb{R}, \quad l = 0, 1, 2, \ldots, \quad r > 0,$$

$$\mathscr{D}(\dot{h}_{\gamma,0}) = \{\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\mathrm{loc}}((0, \infty)); W(\phi, \phi_{\gamma\pm})_{0+} = 0;$$
$$-\phi'' + \gamma r^{-1}\phi \in L^2((0, \infty))\}, \tag{2.1.8}$$
$$\mathscr{D}(\dot{h}_{\gamma,l}) = \{\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\mathrm{loc}}((0, \infty)); -\phi'' + l(l+1)r^{-2}\phi$$
$$+ \gamma r^{-1}\phi \in L^2((0, \infty))\}, \qquad l = 1, 2, \ldots,$$

where

$$\phi_{\gamma\pm}(r) = \mathscr{W}_{-i\gamma/2(\pm i)^{1/2};\,1/2}(-2i(\pm i)^{1/2}r) \text{ and } W(f, g)_x = \overline{f(x)}g'(x) - \overline{f'(x)}g(x)$$

denotes the Wronskain of f and g. As in the case $\gamma = 0$, $\dot{h}_{\gamma,l}$ are self-adjoint for $l \geq 1$ ([389], Ch. X) whereas $\dot{h}_{\gamma,0}$ has deficiency indices (1, 1). By the discussion in Appendix D all self-adjoint extensions $h_{\gamma,0,\alpha}$ of $\dot{h}_{\gamma,0}$ may be parametrized by

$$h_{\gamma,0,\alpha} = -\frac{d^2}{dr^2} + \frac{\gamma}{r}, \qquad \gamma \in \mathbb{R}, \quad r > 0,$$

$$\mathscr{D}(h_{\gamma,0,\alpha}) = \{\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\mathrm{loc}}((0, \infty)); -4\pi\alpha\phi_0 + \phi_1 = 0; \tag{2.1.9}$$
$$-\phi'' + \gamma r^{-1}\phi \in L^2((0, \infty))\}, \qquad -\infty < \alpha \leq \infty,$$

where ϕ_0 and ϕ_1 are defined as

$$\phi_0 = \lim_{r \downarrow 0} \phi(r), \qquad \phi_1 = \lim_{r \downarrow 0} r^{-1}\{\phi(r) - \phi_0[1 + \gamma r \ln(|\gamma| r)]\},$$
$$\phi \in \mathscr{D}(\dot{h}_{\gamma,0}^*), \quad \gamma \in \mathbb{R}. \tag{2.1.10}$$

By an analogous calculation to (1.1.13) one infers that

$$H^c_{\gamma,\theta,y} = T_y^{-1}\left\{\left[U^{-1}h_{\gamma,0,\alpha}U \oplus \bigoplus_{l=1}^{\infty} U^{-1}\dot{h}_{\gamma,l}U\right]\otimes 1\right\}T_y, \qquad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \tag{2.1.11}$$

where

$$\begin{aligned}\alpha = (4\pi)^{-1}(1+e^{i\theta})^{-1}\{[i\gamma((\Psi(1+(i\gamma/2(i)^{1/2})) - \Psi(1) - \Psi(2))/2(i)^{1/2}) - \tfrac{1}{2}]\cdot \\ \cdot(-2i(i)^{1/2}) + e^{i\theta}[i\gamma((\Psi(1+(i\gamma/2(-i)^{1/2})) - \Psi(1) \\ - \Psi(2))/2(-i)^{1/2}) - \tfrac{1}{2}](-2i(-i)^{1/2})\}, \\ (\pm i)^{1/2} = (\pm 1 + i)\cos \pi/4, \quad \gamma \in \mathbb{R}, \end{aligned} \tag{2.1.12}$$

and again α varies in $\mathbb{R}$ ($\alpha = +\infty$ if $\theta \uparrow \pi$) if θ varies in $[0, \pi) \cup (\pi, 2\pi)$. Here $\Psi(\cdot) = \Gamma'(\cdot)/\Gamma(\cdot)$ denotes the digamma function and $\Gamma(\cdot)$ the gamma function [1]. Thus we get

Theorem 2.1.1. *All self-adjoint extensions of $\dot{H}_{\gamma,y}$ are given by*

$$H_{\gamma,\alpha,y} = T_y^{-1}\left\{\left[U^{-1}h_{\gamma,0,\alpha}U \oplus \bigoplus_{l=1}^{\infty} U^{-1}\dot{h}_{\gamma,l}U\right]\otimes 1\right\}T_y,$$
$$-\infty < \alpha \le \infty, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \tag{2.1.13}$$

The special case $\alpha = \infty$ leads to the ordinary Coulomb Hamiltonian $H_{\gamma,y}$ (the Friedrichs extensions of $\dot{H}_{\gamma,y}$) in $L^2(\mathbb{R}^3)$

$$H_{\gamma,y} = -\Delta + \gamma|\cdot - y|^{-1}, \quad \mathscr{D}(H_{\gamma,y}) = H^{2,2}(\mathbb{R}^3), \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \tag{2.1.14}$$

If $|\alpha| < \infty$, $H_{\gamma,\alpha,y}$ describes the Coulomb interaction plus an additional point interaction both centered at $y \in \mathbb{R}^3$. In particular, $H_{\gamma,\alpha,y}$ differs from the Coulomb Hamiltonian $H_{\gamma,y}$ only in the subspace of angular momentum zero, i.e., the point interaction in $H_{\gamma,\alpha,y}$ is again an s-wave ($l = 0$) interaction.

Next we introduce

$$G_{\gamma,k,y} = (H_{\gamma,y} - k^2)^{-1}, \qquad \operatorname{Im} k > 0, \quad k \ne -i\gamma/2n, \quad n = 1, 2, \ldots, \quad \gamma \in \mathbb{R}, \tag{2.1.15}$$

with integral kernel [260]

$$\begin{aligned} G_{\gamma,k,y}(x, x') = \Gamma(1 + (i\gamma/2k))(4\pi|x - x'|)^{-1}\cdot \\ \cdot\left[\left(\frac{d}{d\alpha} - \frac{d}{d\beta}\right)\mathscr{M}_{-i\gamma/2k;\,1/2}(\alpha)\mathscr{W}_{-i\gamma/2k;\,1/2}(\beta)\right]\Bigg|_{\substack{\alpha = -ikx_- \\ \beta = -ikx_+}}, \\ \operatorname{Im} k > 0, \quad k \ne -i\gamma/2n, \quad n = 1, 2, \ldots, \quad \gamma \in \mathbb{R}, \\ x_\pm = |x - y| + |x' - y| \pm |x - x'|, \qquad x, x', y \in \mathbb{R}^3, \quad x \ne x' \end{aligned} \tag{2.1.16}$$

(here $\mathscr{M}_{\mu;\nu}(\cdot)$, $\mathscr{W}_{\mu;\nu}(\cdot)$ denote Whittaker functions [1].)

Basic properties of $H_{\gamma,\alpha,y}$ are described in

Theorem 2.1.2. *Let $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$. The resolvent of $H_{\gamma,\alpha,y}$ is given by*

$$(H_{\gamma,\alpha,y} - k^2)^{-1} = G_{\gamma,k,y} + [\alpha - (\gamma F(i\gamma/2k)/4\pi)]^{-1}(\overline{g_{\gamma,k}(\cdot - y)}, \cdot)g_{\gamma,k}(\cdot - y),$$
$$k^2 \in \rho(H_{\gamma,\alpha,y}), \quad \operatorname{Im} k > 0, \quad (2.1.17)$$

where

$$g_{\gamma,k}(x) = \Gamma(1 + (i\gamma/2k))(4\pi|x|)^{-1}\mathscr{W}_{-i\gamma/2k;\,1/2}(-2ik|x|), \qquad x \neq 0, \quad (2.1.18)$$

and

$$F(i\gamma/2k) = \Psi(1 + (i\gamma/2k)) - \ln(i|\gamma|/2k) + (ik/\gamma) - \Psi(1) - \Psi(2),$$
$$k > 0 \quad \text{or} \quad \operatorname{Im} k > 0, \quad k \neq -i\gamma/2n, \quad n = 1, 2, \ldots. \quad (2.1.19)$$

The domain $\mathscr{D}(H_{\gamma,\alpha,y})$ consists of all elements of the type

$$\psi(x) = \phi_k(x) + [\alpha - (\gamma F(i\gamma/2k)/4\pi)]^{-1}\phi_k(y)g_{\gamma,k}(x - y), \quad (2.1.20)$$

where $\phi_k \in \mathscr{D}(H_{\gamma,y}) = H^{2,2}(\mathbb{R}^3)$ and $k^2 \in \rho(H_{\gamma,\alpha,y})$, $\operatorname{Im} k > 0$. The decomposition (2.1.20) *is unique and with $\psi \in \mathscr{D}(H_{\gamma,\alpha,y})$ of this form we obtain*

$$(H_{\gamma,\alpha,y} - k^2)\psi = (H_{\gamma,y} - k^2)\phi_k. \quad (2.1.21)$$

Next, let $\psi \in \mathscr{D}(H_{\gamma,\alpha,y})$ and assume that $\psi = 0$ in an open set $U \subseteq \mathbb{R}^3$. Then $H_{\gamma,\alpha,y}\psi = 0$ in U.

Proof. Equation (2.1.17) follows from Theorem A.2 except for the factor $[\alpha - (\gamma F(i\gamma/2k)/4\pi)]^{-1}$. In order to determine this factor one can follow the proof of Theorem 1.1.2 by projecting to the subspace of angular momentum zero and replacing $g_0(k, r, r')$, $k^{-1} \sin kr$ and e^{ikr} by the corresponding s-wave Coulomb quantities. The remaining assertions directly follow from Theorem 1.1.3 after replacing G_k, $-\Delta$, $-\Delta_{\alpha,y}$ by $G_{\gamma,k,y}$, $H_{\gamma,y}$, $H_{\gamma,\alpha,y}$, etc. ∎

Spectral properties of $H_{\gamma,\alpha,y}$ are characterized by

Theorem 2.1.3. *Let $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}^3$.*

If $\gamma \geq 0$, then $H_{\gamma,\alpha,y}$ has precisely one negative bound state if $\alpha < -\gamma[\Psi(1) + \Psi(2)]/4\pi$. The eigenvalue $E_0 < 0$ is determined by the equation

$$4\pi\alpha = \gamma\tilde{F}(\gamma/2(-E_0)^{1/2}), \qquad \gamma \geq 0, \quad (2.1.22)$$

with

$$\tilde{F}(\xi) = \Psi(1 + \xi) - \ln|\xi| - (1/2\xi) - \Psi(1) - \Psi(2). \quad (2.1.23)$$

The corresponding strictly positive (unnormalized) eigenfunction is given by $g_{\gamma,i(-E_0)^{1/2}}(x - y)$. If $\alpha \geq -\gamma[\Psi(1) + \Psi(2)]/4\pi$ the point spectrum of $H_{\gamma,\alpha,y}$ is empty.

If $\gamma < 0$, then for all $-\infty < \alpha \leq \infty$ there are always infinitely many simple negative eigenvalues associated with the s-wave ($l = 0$) given by solutions of the equation

$$4\pi\alpha = \gamma\tilde{F}(\gamma/2(-E)^{1/2}), \qquad \gamma < 0. \quad (2.1.24)$$

For angular momenta $l \geq 1$ we get the usual Coulomb levels

$$E_n = -\gamma^2/4n^2, \qquad n = 2, 3, \ldots, \quad \gamma < 0. \tag{2.1.25}$$

For all $\gamma \in \mathbb{R}$ the essential spectrum of $H_{\gamma,\alpha,y}$ is purely absolutely continuous and covers the nonnegative real axis

$$\begin{aligned} &\sigma_{\mathrm{ess}}(H_{\gamma,\alpha,y}) = \sigma_{\mathrm{ac}}(H_{\gamma,\alpha,y}) = [0, \infty), \qquad \sigma_{\mathrm{sc}}(H_{\gamma,\alpha,y}) = \varnothing, \\ &\sigma_{\mathrm{p}}(H_{\gamma,\alpha,y}) \subset (-\infty, 0), \qquad -\infty < \alpha \leq \infty. \end{aligned} \tag{2.1.26}$$

PROOF. Given (2.1.17) the first part of assertions in (2.1.26) then immediately follows from Weyl's theorem ([391], p. 112) and Theorem XIII.20 of [391]. To derive the statements about $\sigma_{\mathrm{p}}(H_{\gamma,\alpha,y}) \cap (-\infty, 0)$ we note the integral representation ([1], p. 259)

$$\tilde{F}(\xi) = -2 \int_0^\infty dt\, t(e^{2\pi t} - 1)^{-1}(t^2 + \xi^2)^{-1} - \Psi(1) - \Psi(2) \tag{2.1.27}$$

implying

$$\tilde{F}(0+) = -\infty, \qquad \tilde{F}(\infty) = -\Psi(1) - \Psi(2), \qquad \tilde{F}'(\xi) > 0, \qquad \xi > 0. \tag{2.1.28}$$

Together with (2.1.17) this proves the assertions for $\gamma \geq 0$. For $\xi < 0$, $\tilde{F}(\xi)$ is strictly increasing from $-\infty$ to $+\infty$ in each interval $(-n-1, -n)$, $n = 0, 1, \ldots$ (cf. Figure 1) which proves the assertions in connection with (2.1.24) and (2.1.25) for $\gamma < 0$. The absence of nonegative eigenvalues follows exactly along the lines of the proof of Theorem 1.1.4. ∎

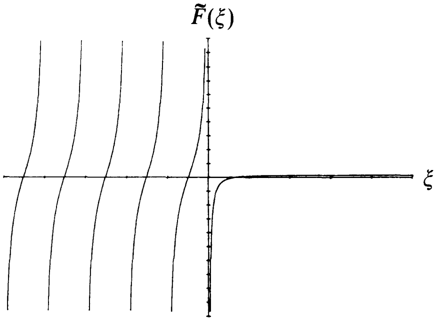


Figure 1 From Albeverio *et al.*, 1983, [22].

Finally, we sketch some properties of complex point interactions. Let $\alpha \in \mathbb{C}$ and define $H_{\gamma,\alpha,y}$ by (2.1.13) (i.e., let $\alpha \in \mathbb{C}$ in (2.1.9)). Then, obviously, $H_{\gamma,\alpha,y}$ is continuous with respect to α in norm resolvent sense. In addition, we have

Theorem 2.1.4. *For all $y \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$, $iH_{\gamma,\alpha,y}$ (resp. $-iH_{\gamma,\alpha,y}$) generates a contraction semigroup $e^{-itH_{\gamma,\alpha,y}}$ (resp. $e^{itH_{\gamma,\alpha,y}}$), $t \geq 0$, in $L^2(\mathbb{R}^3)$ if* $\operatorname{Im} \alpha \leq 0$ *(resp.* $\operatorname{Im} \alpha \geq 0$).

PROOF. From

$$\mathscr{D}(H_{\gamma,\alpha,y}) = \{g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-} | g \in \mathscr{D}(\dot{H}_{\gamma,y}), a \in \mathbb{C}\},$$
$$H_{\gamma,\alpha,y}(g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-}) = \dot{H}_{\gamma,y}g + ia\psi_{\gamma+} - iae^{i\theta}\psi_{\gamma-}, \tag{2.1.29}$$

where α and θ are related by (2.1.12), one infers by a straightforward computation

$$\operatorname{Im}([g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-}], H_{\gamma,\alpha,y}[g + a\psi_{\gamma+} + ae^{i\theta}\psi_{\gamma-}])$$
$$= |a|^2 \|\psi_{\gamma\pm}\|^2(1 - e^{-2\operatorname{Im}\theta}). \tag{2.1.30}$$

Consequently, $\operatorname{Im}(h, H_{\gamma,\alpha,y}h) \le 0$ for all $h \in \mathscr{D}(H_{\gamma,\alpha,y})$ is equivalent to $\operatorname{Im}\theta \le 0$ and hence to $\operatorname{Im}\alpha \le 0$. Thus $iH_{\gamma,\alpha,y}$ is accretive ([389], p. 240) and hence maximal accretive iff $\operatorname{Im}\alpha \le 0$. ∎

I.2.2 Approximations by Means of Scaled Coulomb-Type Interactions

A possible approximation scheme to obtain $H_{\gamma,\alpha,y}$ as the norm resolvent limit of scaled Coulomb-type Hamiltonians is derived in this section. We closely follow the corresponding treatment in Sect. 1.2.

In the following

$$G_{\gamma,k,y} = (H_{\gamma,y} - k^2)^{-1}, \qquad k^2 \in \rho(H_{\gamma,y}), \quad \operatorname{Im} k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \tag{2.2.1}$$

will play the role of an unperturbed resolvent and $V: \mathbb{R}^3 \to \mathbb{R}$ is assumed to be a measurable function belonging to the Rollnik class R. Let u and v be as in Sect. 1.2 (cf. (1.2.3)). Then we have

Lemma 2.2.1. *Let $y \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$, and assume $e^{2a|\cdot|}V \in R$ for some $a > 0$. Then V is form compact with respect to $H_{\gamma,y}$*, i.e.,

$$|V|^{1/2}(|H_{\gamma,y}| + E)^{-1/2} \in \mathscr{B}_\infty(L^2(\mathbb{R}^3)), \qquad E > 0, \tag{2.2.2}$$

and

$$uG_{\gamma,k,y}v \in \mathscr{B}_2(L^2(\mathbb{R}^3)), \quad k \in \Pi_{\gamma,a}, \tag{2.2.3}$$

where

$$\Pi_{\gamma,a} = \{k \in \mathbb{C} | \operatorname{Im} k > -a, k \ne -i\gamma/2n, n = 1, 2, \ldots\}. \tag{2.2.4}$$

PROOF. It suffices to prove (2.2.3). For that purpose we recall the explicit expression [99]

$$\begin{aligned} G_{\gamma,k,y}(x,x') &= (4\pi|x-x'|)^{-1}\{2(x_+ - x_-)^{-1}(x_+x_-)^{-1}F_{\gamma,0}^{(0)}(k, x_-/2)G_{\gamma,0}^{(0)}(-k, x_+/2) \\ &\quad - 3^{-1}(k^2 + (\gamma^2/4))F_{\gamma,1}^{(0)}(k, x_-/2)G_{\gamma,0}^{(0)}(-k, x_+/2) \\ &\quad + 3F_{\gamma,0}^{(0)}(k, x_-/2)G_{\gamma,1}^{(0)}(-k, x_+/2)\} \\ &= (4\pi|x-x'|)^{-1}\{2(x_+ - x_-)(x_+x_-)^{-1}F_{\gamma,0}^{(0)}(k, x_-/2)\tilde{G}_{\gamma,0}^{(0)}(k, x_+/2) \\ &\quad - 3^{-1}(k^2 + (\gamma^2/4))F_{\gamma,1}^{(0)}(k, x_-/2)\tilde{G}_{\gamma,0}^{(0)}(k, x_+/2) \end{aligned}$$

$$+ 3F_{\gamma,0}^{(0)}(k, x_-/2)\tilde{G}_{\gamma,1}^{(0)}(k, x_+/2)\}$$
$$+ (4\pi|x - x'|)^{-1}\gamma[\Psi(1 + (i\gamma/2k)) - \ln(i|\gamma|/2k) + (ik/\gamma)] \cdot$$
$$\cdot \{2(x_+ - x_-)(x_+x_-)^{-1}F_{\gamma,0}^{(0)}(k, x_-/2)F_{\gamma,0}^{(0)}(k, x_+/2)$$
$$- 3^{-1}(k^2 + (\gamma^2/4))[F_{\gamma,1}^{(0)}(k, x_-/2)F_{\gamma,0}^{(0)}(k, x_+/2)$$
$$- F_{\gamma,0}^{(0)}(k, x_-/2)F_{\gamma,1}^{(0)}(k, x_+/2)]\},$$
$$k \in \Pi_{\gamma,\infty}, \quad x \neq x', \quad x_\pm = |x - y| + |x' - y| \pm |x - x'|, \quad (2.2.5)$$

where

$$F_{\gamma,l}^{(0)}(k, r) = r^{l+1}e^{ikr}{}_1F_1(l + 1 + (i\gamma/2k); 2l + 2; -2ikr),$$
$$G_{\gamma,l}^{(0)}(-k, r) = \Gamma(2l + 2)^{-1}\Gamma(l + 1 + (i\gamma/2k))(2ie^{-i\pi}k)^{2l+1}r^{l+1}e^{ikr} \cdot$$
$$\cdot U(l + 1 + (i\gamma/2k); 2l + 2; 2ie^{-i\pi}kr), \quad (2.2.6)$$
$$\tilde{G}_{\gamma,l}^{(0)}(k, r) = G_{\gamma,l}^{(0)}(-k, r) - 2^{2l}\Gamma(2l + 2)^{-2}|\Gamma(1 + (i\gamma/2k))|^{-2}|\Gamma(l + 1 + (i\gamma/2k))|^2 \cdot$$
$$\cdot \gamma k^{2l}[\Psi(1 + (i\gamma/2k)) - \ln(i|\gamma|/2k) + (ik/\gamma)]F_{\gamma,l}^{(0)}(k, r); \qquad l = 0, 1,$$

and ${}_1F_1(\alpha; \beta; \cdot)$, $(U(\alpha; \beta; \cdot))$ denotes the (ir)regular confluent hypergeometric function [1]. In fact, the bound [96], [99]

$$|H_{\gamma,l}^{(0)}(k, r)| \leq \text{const}(\varepsilon, \gamma, \kappa_0, R_0)\exp\{(1 + \varepsilon)\kappa_0(r - R_0) + (|\gamma|/2\kappa_0)\ln(r/R_0)\},$$
$$\varepsilon > 0, \quad \gamma \in \mathbb{R}, \quad \kappa_0 > 0, \quad |k^2| \leq \kappa_0^2, \quad r \geq R_0 > 0, \quad l = 0, 1, \quad (2.2.7)$$

where $H_{\gamma,l}^{(0)}$ denotes $F_{\gamma,l}^{(0)}$, $(\partial/\partial(k^2))F_{\gamma,l}^{(0)}$, $\tilde{G}_{\gamma,l}^{(0)}$, or $(\partial/\partial(k^2))\tilde{G}_{\gamma,l}^{(0)}$, $l = 0, 1$, together with the second equality in (2.2.5) proves that $uG_{\gamma,k,y}v \in \mathscr{B}_2(L^2(\mathbb{R}^3))$ for $k \in \Pi_{\gamma,a}$, $|k| < a$. The asymptotic behavior [1]

$$F_{\gamma,l}^{(0)}(k, r) \underset{r\to\infty}{\overset{|k|>0}{\approx}} e^{-ikr}\{r^{i\gamma/2k}c_1(l, \gamma, k) + O(r^{-1})\} + e^{ikr}\{r^{-i\gamma/2k}c_2(l, \gamma, k) + O(r^{-1})\},$$

$$G_{\gamma,l}^{(0)}(-k, r) \underset{r\to\infty}{\overset{|k|>0}{\approx}} e^{ikr}\{r^{-i\gamma/2k}c_3(l, \gamma, k) + O(r^{-1})\}; \qquad k \in \Pi_{\gamma,\infty}, \quad (2.2.8)$$

for appropriate coefficients c_j, $j = 1, 2, 3$, together with the first equality in (2.2.5) and with (2.2.7) then proves $uG_{\gamma,k,y}v \in \mathscr{B}_2(L^2(\mathbb{R}^3))$ for $k \in \Pi_{\gamma,a}$. For Im $k > 0$ this also directly follows from the bound (4.1) of [231]

$$|G_{\gamma,k,y}(x, x')| \leq C_\gamma(k)|x - x'|^{-1}e^{-(\mathrm{Im}\,k)|x-x'|}[1 + |x - x'|]^{-\theta(-\gamma)\gamma\,\mathrm{Im}\,k/2|k|^2},$$
$$k \in \Pi_{\gamma,0}, \qquad x \neq x'. \quad (2.2.9)$$

■

Next we recall

$$\tilde{v}(x) = v(x - \varepsilon^{-1}y), \qquad \tilde{u}(x) = u(x - \varepsilon^{-1}y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3, \quad (2.2.10)$$

and introduce

$$\tilde{B}(\varepsilon, \gamma\,\varepsilon\ln\varepsilon, k) = \lambda(\varepsilon, \gamma\,\varepsilon\ln\varepsilon)\tilde{u}G_{\varepsilon\gamma,k,y/\varepsilon}\tilde{v}, \qquad \varepsilon > 0, \quad k \in \Pi_{\gamma,0}, \quad (2.2.11)$$

where $\lambda(\cdot, \cdot)$ is real analytic near the origin with

$$\lambda(\varepsilon, \gamma\varepsilon\ln\varepsilon) = \sum_{m,n=0}^{\infty} \lambda_{mn}\varepsilon^m(\gamma\varepsilon\ln\varepsilon)^n, \qquad \lambda_{00} = 1. \quad (2.2.12)$$

Because of (2.2.3), $\tilde{B}(\varepsilon, \gamma\varepsilon \ln \varepsilon, k)$ extends to a Hilbert–Schmidt operator for $k \in \Pi_{\gamma,a}$. Moreover, by (2.2.2) and the discussion in Appendix B the form sum

$$H_{\varepsilon\gamma, y/\varepsilon}(\varepsilon) = -\Delta + \varepsilon\gamma |x - \varepsilon^{-1} y|^{-1} \dot{+} \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) V(\cdot - \varepsilon^{-1} y),$$
$$\varepsilon > 0, \quad y \in \mathbb{R}^3, \quad (2.2.13)$$

is well defined and the resolvent equation

$$(H_{\varepsilon\gamma, y/\varepsilon}(\varepsilon) - k^2)^{-1}$$
$$= G_{\varepsilon\gamma,k,y/\varepsilon} - \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) G_{\varepsilon\gamma,k,y/\varepsilon} \tilde{v}[1 + \tilde{B}(\varepsilon, \gamma\varepsilon \ln \varepsilon, k)]^{-1} \tilde{u} G_{\varepsilon\gamma,k,y/\varepsilon},$$
$$\varepsilon > 0, \quad k^2 \in \rho(H_{\varepsilon\gamma,y}(\varepsilon)), \quad k \in \Pi_{\varepsilon\gamma,0}, \quad y \in \mathbb{R}^3, \quad (2.2.14)$$

holds. Following Sect. 1.2 we define

$$\begin{aligned} H_{\gamma,\varepsilon,y} &= \varepsilon^{-2} U_\varepsilon H_{\varepsilon\gamma,y/\varepsilon}(\varepsilon) U_\varepsilon^{-1} = H_{\gamma,y} \dot{+} V_{\varepsilon,y}, \\ V_{\varepsilon,y}(x) &= \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon)\varepsilon^{-2} V((x - y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3, \end{aligned} \quad (2.2.15)$$

where U_ε denotes the unitary scaling group (1.2.10) in $L^2(\mathbb{R}^3)$. Since we are interested in the limit $\varepsilon \downarrow 0$ of $H_{\gamma,\varepsilon,y}$ we first introduce Hilbert–Schmidt operators $A_{\gamma,\varepsilon}(k)$, $B_{\gamma,\varepsilon}(k) = \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) u G_{\varepsilon\gamma,\varepsilon k} v$, $C_{\gamma,\varepsilon}(k)$, $0 < \varepsilon < \varepsilon_0$, with integral kernels

$$A_{\gamma,\varepsilon}(k, x, x') = G_{\gamma,k}(x - y, \varepsilon x') v(x'), \qquad k \in \Pi_{\gamma,0}, \quad (2.2.16)$$

$$B_{\gamma,\varepsilon}(k, x, x') = \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) u(x) G_{\varepsilon\gamma,\varepsilon k}(x, x') v(x'), \qquad k \in \Pi_{\gamma,a/\varepsilon_0}, \quad (2.2.17)$$

$$C_{\gamma,\varepsilon}(k, x, x') = u(x) G_{\gamma,k}(\varepsilon x, x' - y), \qquad k \in \Pi_{\gamma,0}, \quad (2.2.18)$$

where we abbreviate

$$G_{\gamma,k,0}(x, x') = G_{\gamma,k}(x, x'), \qquad x \neq x'. \quad (2.2.19)$$

From the scaling behavior

$$\varepsilon^2 U_\varepsilon G_{\gamma,k,y} U_\varepsilon^{-1} = G_{\gamma/\varepsilon, k/\varepsilon, \varepsilon y}, \qquad \varepsilon > 0, \quad k \in \Pi_{\gamma,0}, \quad y \in \mathbb{R}^3, \quad (2.2.20)$$

we infer from (2.2.14) after a translation $x \to x + (y/\varepsilon)$, $\varepsilon > 0$,

$$\begin{aligned} (H_{\gamma,\varepsilon,y} - k^2)^{-1} &= \varepsilon^2 U_\varepsilon [H_{\varepsilon\gamma,y/\varepsilon}(\varepsilon) - (\varepsilon k)^2]^{-1} U_\varepsilon^{-1} \\ &= G_{\gamma,k,y} - \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) A_{\gamma,\varepsilon}(k) \varepsilon [1 + B_{\gamma,\varepsilon}(k)]^{-1} C_{\gamma,\varepsilon}(k), \end{aligned}$$
$$\varepsilon > 0, \quad k^2 \in \rho(H_{\gamma,\varepsilon,y}), \quad k \in \Pi_{\gamma,0}, \quad y \in \mathbb{R}^3. \quad (2.2.21)$$

Lemma 2.2.2. *Let $y \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$, and define rank-one operators $A_\gamma(k)$, $C_\gamma(k)$, and the Hilbert–Schmidt operator uG_0v with integral kernels*

$$A_\gamma(k, x, x') = G_{\gamma,k}(x - y, 0) v(x'), \qquad k \in \Pi_{\gamma,0}, \quad x \neq y, \quad (2.2.22)$$

$$uG_0v(x, x') = u(x)(4\pi |x - x'|)^{-1} v(x'), \qquad x \neq x', \quad (2.2.23)$$

$$C_\gamma(k, x, x') = u(x) G_{\gamma,k}(0, x' - y), \qquad k \in \Pi_{\gamma,0}, \quad x' \neq y. \quad (2.2.24)$$

Then, for fixed $k \in \Pi_{\gamma,0}$, $A_{\gamma,\varepsilon}(k)$, $B_{\gamma,\varepsilon}(k)$, $C_{\gamma,\varepsilon}(k)$ converge in Hilbert–Schmidt norm to $A_\gamma(k)$, uG_0v, $C_\gamma(k)$, respectively, as $\varepsilon \downarrow 0$.

Proof. Using the bound (2.2.9) [231] one can follow the proof of Lemma 1.2.2 step by step. ■

As in the short-range case $\gamma = 0$, it remains to determine the limit of $\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1}$ as $\varepsilon \downarrow 0$. Because of $\text{n-lim}_{\varepsilon\downarrow 0}[1 + B_{\gamma,\varepsilon}(k)] = (1 + uG_0v)$ again the zero-energy properties of $H = -\Delta \dotplus V$ enter at this point. We first formulate

Lemma 2.2.3. *Let $\gamma \in \mathbb{R}$ and $e^{2a|\cdot|}V \in R$ for some $a > 0$. Then $B_{\gamma,\varepsilon}(k)$, $0 < \varepsilon < \varepsilon_0$, $k \in \Pi_{\gamma, a/\varepsilon_0}$, is (norm) analytic with respect to $(\varepsilon, \gamma\varepsilon \ln \varepsilon)$ near the origin*

$$B_{\gamma,\varepsilon}(k) = \sum_{m,n=0}^{\infty} B_{mn}(\gamma, k)\varepsilon^m(\gamma\varepsilon \ln \varepsilon)^n. \tag{2.2.25}$$

The coefficients $B_{mn}(\gamma, k)$, $m, n = 0, 1, \ldots,$ are Hilbert–Schmidt operators and the first few of them explicitly read

$$B_{00} = uG_0v, \tag{2.2.26}$$

$$\begin{aligned} B_{10}(\gamma, k) = \lambda_{10}uG_0v &+ \gamma(4\pi)^{-1}F(i\gamma/2k)(v, \cdot)u \\ &+ \gamma(4\pi)^{-1}u \ln(|\gamma|x_+/2)v, \end{aligned} \tag{2.2.27}$$

$$B_{01} = \lambda_{01}uG_0v + (4\pi)^{-1}(v, \cdot)u, \tag{2.2.28}$$

where $u \ln(|\gamma|x_+/2)v$ has the integral kernel

$$u(x)\ln[|\gamma|(|x| + |x'| + |x - x'|)/2]v(x'). \tag{2.2.29}$$

Proof. By the first equality in (2.2.5) and the series expansions [1]

$$\begin{aligned}
&{}_1F_1(l + 1 + (i\gamma/2k); 2l + 2; -i\varepsilon k x_-) \\
&\quad = \sum_{n=0}^{\infty} \frac{\Gamma(n + l + 1 + (i\gamma/2k))\Gamma(2l + 2)(-i\varepsilon k x_-)^n}{\Gamma(l + 1 + (i\gamma/2k))\Gamma(n + 2l + 2)\Gamma(n + 1)}, \\
&U(l + 1 + (i\gamma/2k), 2l + 2; ie^{-i\pi}\varepsilon k x_+) \\
&\quad = \Gamma(2l+2)^{-1}\Gamma(-l+(i\gamma/2k))^{-1}\{{}_1F_1(l+1+(i\gamma/2k); 2l+2; -i\varepsilon k x_+)\ln(ie^{-i\pi}\varepsilon k x_+) \\
&\qquad + \sum_{n=0}^{\infty} \frac{\Gamma(n + l + 1 + (i\gamma/2k))\Gamma(2l + 2)(-i\varepsilon k x_+)^n}{\Gamma(l + 1 + (i\gamma/2k))\Gamma(n + 2l + 2)\Gamma(n + 1)} \cdot \\
&\qquad \cdot[\Psi(n + l + 1 + (i\gamma/2k)) - \Psi(n + 2l + 2) - \Psi(n + 1)]\} \\
&\qquad + \frac{\Gamma(2l + 1)}{\Gamma(l + 1 + (i\gamma/2k))}\,{}_1F_1(-l + (i\gamma/2k); -2l; -i\varepsilon k x_+)_{2l+1};
\end{aligned}$$

$$k \in \Pi_{\gamma,\infty}, \quad l = 0, 1, \tag{2.2.30}$$

one infers that the integral kernel of $G_{\varepsilon\gamma,\varepsilon k}$

$$G_{\varepsilon\gamma,\varepsilon k}(x, x') = \sum_{m=0}^{\infty} \hat{G}_{m0}(\gamma, k, x, x')\varepsilon^m + (\gamma\varepsilon \ln \varepsilon) \sum_{m=0}^{\infty} \hat{G}_{m1}(\gamma, k, x, x')\varepsilon^m,$$

$$k \in \Pi_{\gamma,\infty}, \quad x \neq x', \tag{2.2.31}$$

is analytic in $(\varepsilon, \gamma\varepsilon \ln \varepsilon)$ near $(0, 0)$ and that $|x - x'| \hat{G}_{mn}(\gamma, k, x, x')$, $m = 0, 1, \ldots, n = 0$ or 1, are polynomially bounded in $|x|$ and $|x'|$. Thus taking matrix elements with $C_0^\infty(\mathbb{R}^3)$ functions we get analyticity of $uG_{\varepsilon\gamma,\varepsilon k}v$ and hence of $B_{\gamma,\varepsilon}(k)$ in $(\varepsilon, \gamma\varepsilon \ln \varepsilon)$ near the origin. ∎

Given the case distinction I–IV of Sect. 1.2 (and the ordering $(v, \phi_1) \neq 0$, $(v, \phi_l) = 0$, $l = 2, \ldots, N$, in case IV) we have

Lemma 2.2.4. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$, $0 < \varepsilon < \varepsilon_0$ small enough and assume case* I *(i.e., $P = 0$). Then $\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1}$, $\gamma \in \mathbb{R}$, is analytic in $(\varepsilon, \gamma\varepsilon \ln \varepsilon)$ near the origin and we get the norm convergent expansion*

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} = \varepsilon[(1 + uG_0v)^{-1} - \varepsilon(1 + uG_0v)^{-1}B_{10}(\gamma, k)(1 + uG_0v)^{-1} - (\gamma\varepsilon \ln \varepsilon)(1 + uG_0v)^{-1}B_{01}(1 + uG_0v)^{-1} + O((\varepsilon \ln \varepsilon)^2)],$$
$$k \in \Pi_{\gamma, a/\varepsilon_0}. \quad (2.2.32)$$

PROOF. Since $(1 + uG_0v)^{-1} \in \mathscr{B}(L^2(\mathbb{R}^3))$, (2.2.32) immediately follows from

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} = \varepsilon\{1 + (1 + uG_0v)^{-1}[\varepsilon B_{10} + (\gamma\varepsilon \ln \varepsilon)B_{01} + O((\varepsilon \ln \varepsilon)^2)]\}^{-1}(1 + uG_0v)^{-1}. \quad (2.2.33)$$

∎

Lemma 2.2.5. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$, $0 < \varepsilon < \varepsilon_0$ small enough and assume case* II *(i.e., $P = -(\tilde{\phi}, \cdot)\phi$, $(v, \phi) \neq 0$).*

(i) *If $\lambda_{01} = -|(v, \phi)|^2/4\pi$ we get the norm convergent expansion*

$$\begin{aligned}\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} &= \langle B_{10}\rangle^{-1}(\tilde{\phi}, \cdot)\phi + \varepsilon T \\ &- \varepsilon\langle B_{10}\rangle^{-1}[(T^*B_{10}^*\tilde{\phi}, \cdot)\phi + (\tilde{\phi}, \cdot)TB_{10}\phi] \\ &- (\gamma\varepsilon \ln \varepsilon)\langle B_{10}\rangle^{-1}[(T^*B_{01}^*\tilde{\phi}, \cdot)\phi + (\tilde{\phi}, \cdot)TB_{01}\phi] \\ &- \langle B_{10}\rangle^{-2}[\varepsilon\langle B_{20}\rangle + (\gamma\varepsilon \ln \varepsilon)\langle B_{11}\rangle + \varepsilon(\gamma \ln \varepsilon)^2\langle B_{02}\rangle](\tilde{\phi}, \cdot)\phi \\ &+ \langle B_{10}\rangle^{-2}\{\varepsilon\langle B_{10}TB_{10}\rangle + (\gamma\varepsilon \ln \varepsilon)[\langle B_{10}TB_{01}\rangle + \langle B_{01}TB_{10}\rangle] \\ &+ \varepsilon(\gamma \ln \varepsilon)^2\langle B_{01}TB_{01}\rangle\}(\tilde{\phi}, \cdot)\phi + O(\varepsilon^2(\ln \varepsilon)^3),\end{aligned}$$
$$k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R}. \quad (2.2.34)$$

(ii) *If $\lambda_{01} \neq -|(v, \phi)|^2/4\pi$ we get the norm convergent expansion*

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} = (\gamma \ln \varepsilon)^{-1}\langle B_{01}\rangle^{-1}(\tilde{\phi}, \cdot)\phi - (\gamma \ln \varepsilon)^{-2}\langle B_{01}\rangle^{-2}\langle B_{10}\rangle(\tilde{\phi}, \cdot)\phi + O((\ln \varepsilon)^{-3}),$$
$$k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.2.35)$$

Here we used the notation $\langle B\rangle = (\tilde{\phi}, B\phi)$ for bounded operators $B \in \mathscr{B}(L^2(\mathbb{R}^3))$ and suppressed the γ and k dependence in $B_{mn}(\gamma, k)$.

PROOF. Define

$$B(\gamma, \varepsilon, k) = B_{\gamma,\varepsilon}(k) - B_{00}, \qquad k \in \Pi_{\gamma,a/\varepsilon_0}, \tag{2.2.36}$$

and let $\mu \in \mathbb{C} - \{0\}$, $|\mu|$ small enough. Then (1.2.35) implies

$$\begin{aligned}\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} &= \varepsilon\{1 + (1 + B_{00} + \mu)^{-1}[B(\varepsilon) - \mu]\}^{-1}(1 + B_{00} + \mu)^{-1} \\ &= \varepsilon\{PB(\varepsilon) + \mu - \mu P + \mu TB(\varepsilon) + O(\mu^2)\}^{-1}[P + \mu T + O(\mu^2)] \\ &= \varepsilon\{1 + \mu(PB(\varepsilon) + \mu)^{-1}[-P + TB(\varepsilon) + O(\mu)]\}^{-1} \cdot \\ &\quad \cdot [PB(\varepsilon) + \mu]^{-1}[P + \mu T + O(\mu^2)]. \end{aligned} \tag{2.2.37}$$

From $P = -(\tilde{\phi}, \cdot)\phi$ we get

$$\mu[PB(\varepsilon) + \mu]^{-1} = 1 - \langle [B(\varepsilon) + \mu] \rangle^{-1}(B(\varepsilon)^*\tilde{\phi}, \cdot)\phi \tag{2.2.38}$$

and thus

$$\begin{aligned}\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} &= \varepsilon\{1 + TB(\varepsilon) - \langle B(\varepsilon)\rangle^{-1}(B(\varepsilon)^*T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi + O(\mu)\}^{-1} \cdot \\ &\quad \cdot [\langle B(\varepsilon)\rangle^{-1}(\tilde{\phi}, \cdot)\phi + T - \langle B(\varepsilon)\rangle^{-1}(T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi + O(\mu)]. \end{aligned} \tag{2.2.39}$$

Since $\mu \neq 0$ was arbitrary we get

$$\begin{aligned}\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} &= \{1 + TB(\varepsilon) - \langle B(\varepsilon)\rangle^{-1}(B(\varepsilon)^*T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi\}^{-1} \cdot \\ &\quad \cdot \varepsilon[\langle B(\varepsilon)\rangle^{-1}(\tilde{\phi}, \cdot)\phi + T - \langle B(\varepsilon)\rangle^{-1}(T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi] \\ &= \{1 - TB(\varepsilon) + \langle B(\varepsilon)\rangle^{-1}(B(\varepsilon)^*T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi + O(\varepsilon^2(\ln \varepsilon)^3)\} \cdot \\ &\quad \cdot \varepsilon[\langle B(\varepsilon)\rangle^{-1}(\tilde{\phi}, \cdot)\phi + T - \langle B(\varepsilon)\rangle^{-1}(T^*B(\varepsilon)^*\tilde{\phi}, \cdot)\phi]. \end{aligned} \tag{2.2.40}$$

Now assume $\lambda_{01} = -|(v, \phi)|^2/4\pi$ which is equivalent to $\langle B_{01}\rangle = 0$. Then

$$\begin{aligned}\langle B(\varepsilon)\rangle^{-1} &= \varepsilon^{-1}\langle B_{10}\rangle^{-1}\{1 - \langle B_{10}\rangle^{-1}[\varepsilon\langle B_{20}\rangle + (\gamma\varepsilon \ln \varepsilon)\langle B_{11}\rangle \\ &\quad + \varepsilon(\gamma \ln \varepsilon)^2\langle B_{02}\rangle] + O(\varepsilon^2(\ln \varepsilon)^3)\} \end{aligned} \tag{2.2.41}$$

and we obtain (2.2.34). If $\lambda_{01} \neq -|(v, \phi)|^2/4\pi$ (i.e., $\langle B_{01}\rangle \neq 0$) then

$$\langle B(\varepsilon)\rangle^{-1} = (\gamma\varepsilon \ln \varepsilon)^{-1}\langle B_{01}\rangle^{-1}[1 - (\gamma \ln \varepsilon)^{-1}\langle B_{01}\rangle^{-1}\langle B_{10}\rangle + O((\ln \varepsilon)^{-2})] \tag{2.2.42}$$

implies (2.2.35). ■

Lemma 2.2.6. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$, $0 < \varepsilon < \varepsilon_0$ small enough and assume case* III *(i.e., $P = -\sum_{l=1}^{N}(\tilde{\phi}_l, \cdot)\phi_l$, $(v, \phi_l) = 0$, $l = 1, \ldots, N$).*

(i) *If $\lambda_{01} = 0$ and the matrix $(\tilde{\phi}_l, B_{10}(\gamma, k)\phi_{l'})$, $l, l' = 1, \ldots, N$, is nonsingular we get the expansion valid in norm*

$$\begin{aligned}&\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} \\ &= \sum_{l,l'=1}^{N} (\langle B_{10}\rangle)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l + \varepsilon T \\ &\quad - \varepsilon \sum_{l,l'=1}^{N} (\langle B_{10}\rangle)_{ll'}^{-1}[(TB_{10}^*\tilde{\phi}_{l'}, \cdot)\phi_l + (\tilde{\phi}_{l'}, \cdot)TB_{10}\phi_l]\end{aligned}$$

$$
\begin{aligned}
&-(\gamma\varepsilon \ln \varepsilon) \sum_{l,l'=1}^{N} (\langle B_{10}\rangle)_{ll'}^{-1}[(T^* B_{01}^* \tilde{\phi}_{l'}, \cdot)\phi_l + (\tilde{\phi}_{l'}, \cdot) T B_{01}\phi_l] \\
&+ \sum_{l,l',l'',l'''=1}^{N} (\langle B_{10}\rangle)_{ll''}^{-1}[\varepsilon\langle B_{10}^2\rangle_{l',l''} \\
&+ (\gamma\varepsilon \ln \varepsilon)\langle [B_{10}B_{01} + B_{01}B_{10}]\rangle_{l'l''} + \varepsilon(\gamma \ln \varepsilon)^2 \langle B_{01}^2\rangle_{l'l''}] \cdot \\
&\cdot (\langle B_{10}\rangle)_{l''l'''}^{-1}(\tilde{\phi}_{l'''}, \cdot)\phi_l + \sum_{l,l',l'',l'''=1}^{N} (\langle B_{10}\rangle)_{ll''}^{-1}[\varepsilon\langle B_{20}\rangle_{l''l'''} \\
&+ (\gamma\varepsilon \ln \varepsilon)\langle B_{11}\rangle_{l''l'''} + \varepsilon(\gamma \ln \varepsilon)^2\langle B_{02}\rangle_{l''l'''}] \cdot \\
&\cdot (\langle B_{10}\rangle)_{l'''l'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l + O(\varepsilon^2(\ln \varepsilon)^3), \qquad k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R}.
\end{aligned} \tag{2.2.43}
$$

(ii) *If $\lambda_{01} \neq 0$, we obtain the expansion valid in norm*

$$
\begin{aligned}
&\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} \\
&= (\gamma \ln \varepsilon)^{-1} \sum_{l,l'=1}^{N} (\langle B_{01}\rangle)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l \\
&\quad - (\gamma \ln \varepsilon)^{-2} \sum_{l,l',l'',l'''=1}^{N} (\langle B_{01}\rangle)_{ll''}^{-1}\langle B_{10}\rangle_{l''l'''}(\langle B_{01}\rangle)_{l'''l'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l \\
&\quad + O((\ln \varepsilon)^{-3}), \qquad k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R} - \{0\}.
\end{aligned} \tag{2.2.44}
$$

Here we used $\langle B\rangle_{ll'} = (\tilde{\phi}_l, B\phi_{l'})$ and $(\langle B\rangle)_{ll'}^{-1}$ *the inverse matrix of $\langle B\rangle_{ll'}$ for some $B \in \mathscr{B}(L^2(\mathbb{R}^3))$.*

PROOF. Inserting

$$
\mu[PB(\varepsilon) + \mu]^{-1} = 1 - \sum_{l,l'=1}^{N} (\langle B(\varepsilon) + \mu\rangle)_{ll'}^{-1}(B(\varepsilon)^*\tilde{\phi}_{l'}, \cdot)\phi_l \tag{2.2.45}
$$

into (2.2.37) one arrives after some manipulations at

$$
\begin{aligned}
\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} = &\left\{1 - TB(\varepsilon) + \sum_{l,l'=1}^{N} (\langle B(\varepsilon)\rangle)_{ll'}^{-1}(B(\varepsilon)^* T^* B(\varepsilon)^*\tilde{\phi}_{l'}, \cdot)\phi_l \right. \\
&\left. + O(\varepsilon^2(\ln \varepsilon)^3)\right\}\varepsilon\left[\sum_{l,l'=1}^{N} (\langle B(\varepsilon)\rangle)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l + T \right. \\
&\left. - \sum_{l,l'=1}^{N} (\langle B(\varepsilon)\rangle)_{ll'}^{-1}(T^* B(\varepsilon)^*\tilde{\phi}_{l'}, \cdot)\phi_l\right].
\end{aligned} \tag{2.2.46}
$$

Now assume $\lambda_{01} = 0$ and $\langle B_{10}\rangle_{ll'}$ to be nonsingular. Then

$$
\begin{aligned}
\varepsilon(\langle B(\varepsilon)\rangle)_{ll'}^{-1} = (\langle B_{10}\rangle)_{ll'}^{-1} - &\sum_{l'',l'''=1}^{N} (\langle B_{10}\rangle)_{ll''}^{-1}[\varepsilon\langle B_{20}\rangle_{l''l'''} + (\gamma\varepsilon \ln \varepsilon)\langle B_{11}\rangle_{l''l'''} \\
&+ \varepsilon(\gamma \ln \varepsilon)^2\langle B_{02}\rangle_{l''l'''}](\langle B_{10}\rangle)_{l'''l'}^{-1} + O(\varepsilon^2(\ln \varepsilon)^3)
\end{aligned} \tag{2.2.47}
$$

and (2.2.43) follows. On the other hand, if $\lambda_{01} \neq 0$, then

$$\varepsilon(\langle B(\varepsilon)\rangle)_{ll'}^{-1} = (\gamma \ln \varepsilon)^{-1}(\langle B_{01}\rangle)_{ll'}^{-1}$$
$$- (\gamma \ln \varepsilon)^{-2} \sum_{l'',l'''=1}^{N} (\langle B_{01}\rangle)_{ll''}^{-1}\langle B_{10}\rangle_{l''l'''}(\langle B_{01}\rangle)_{l'''l'}^{-1} + O((\ln \varepsilon)^{-3}), \tag{2.2.48}$$

which proves (2.2.44). ■

Lemma 2.2.7. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$, $0 < \varepsilon < \varepsilon_0$ small enough and assume case* IV *and* (1.2.84) (*i.e.*, $P = -\sum_{l=1}^{N} (\tilde{\phi}_l, \cdot)\phi_l$, $(v, \phi_1) \neq 0$, $(v, \phi_l) = 0$, $l = 2, \ldots, N$).

(i) *If $\lambda_{01} = -|(v, \phi_l)|^2/4\pi$ we get the expansion valid in norm*

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1}$$
$$= \langle B_{10}\rangle_{11}^{-1}(\tilde{\phi}_1, \cdot)\phi_1 + (\lambda_{01}\gamma \ln \varepsilon)^{-1} \sum_{l=2}^{N} (\tilde{\phi}_l, \cdot)\phi_l$$
$$- (\lambda_{01}\gamma \ln \varepsilon)^{-1}\langle B_{10}\rangle_{11}^{-1} \sum_{l=2}^{N} [\langle B_{10}\rangle_{1l}(\tilde{\phi}_l, \cdot)\phi_1 + \langle B_{10}\rangle_{l1}(\tilde{\phi}_1, \cdot)\phi_l]$$
$$+ (\lambda_{01}\gamma \ln \varepsilon)^{-1}\langle B_{10}\rangle_{11}^{-2} \sum_{l=2}^{N} |\langle B_{10}\rangle_{1l}|^2(\tilde{\phi}_1, \cdot)\phi_1 + O((\ln \varepsilon)^{-2}),$$
$$k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R} - \{0\}. \tag{2.2.49}$$

(ii) *If $\lambda_{01} \neq -|(v, \phi_1)|^2/4\pi$ we get the expansion valid in norm*

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1}$$
$$= (\gamma \ln \varepsilon)^{-1} \sum_{l,l'=1}^{N} (\langle B_{01}\rangle)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l$$
$$- (\gamma \ln \varepsilon)^{-2} \sum_{l,l',l'',l'''=1}^{N} (\langle B_{01}\rangle)_{ll''}^{-1}\langle B_{10}\rangle_{l''l'''}(\langle B_{01}\rangle)_{l'''l'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l$$
$$+ O((\ln \varepsilon)^{-3}), \qquad k \in \Pi_{\gamma, a/\varepsilon_0}, \quad \gamma \in \mathbb{R} - \{0\}. \tag{2.2.50}$$

PROOF. From (2.2.46) we get

$$\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} = \sum_{l,l'=1}^{N} (\langle B_{10} + (\gamma \ln \varepsilon)B_{01}\rangle)_{ll'}^{-1}(\tilde{\phi}_{l'}, \cdot)\phi_l + O(\varepsilon(\ln \varepsilon)^2). \tag{2.2.51}$$

If the matrix $\langle B_{01}\rangle_{ll'}$ is singular, or equivalently if $\lambda_{01} = -|(v, \phi_1)|^2/4\pi$, then

$$(\langle B_{10} + \gamma \ln \varepsilon B_{01}\rangle)_{ll'}^{-1}$$
$$= \langle B_{10}\rangle_{11}^{-1}\delta_{l1}\delta_{l'1} + (\lambda_{01}\gamma \ln \varepsilon)^{-1}[\delta_{ll'} - \delta_{l1}\delta_{l'1}]$$
$$- (\lambda_{01}\gamma \ln \varepsilon)^{-1}\langle B_{10}\rangle_{11}^{-1}[\delta_{l1}\langle B_{10}\rangle_{1l'}(1 - \delta_{l'1}) + (1 - \delta_{l1})\langle B_{10}\rangle_{l1}\delta_{l'1}]$$
$$- (\lambda_{01}\gamma \ln \varepsilon)^{-1}\langle B_{10}\rangle_{11}^{-2} \sum_{l''=2}^{N} |\langle B_{10}\rangle_{1l''}|^2\delta_{l1}\delta_{l'1} + O((\ln \varepsilon)^{-2}) \tag{2.2.52}$$

and (2.2.49) follows. If $\langle B_{01}\rangle_{ll'}$ is nonsingular, i.e., if $\lambda_{01} \neq -|(v, \phi_1)|^2/4\pi$, then

$$\begin{aligned}(\langle B_{10} + (\gamma \ln \varepsilon)B_{01}\rangle)_{ll'}^{-1} &= (\gamma \ln \varepsilon)^{-1}(\langle B_{01}\rangle)_{ll'}^{-1} \\ &\quad - (\gamma \ln \varepsilon)^{-2} \sum_{l'',l'''=1}^{N} (\langle B_{01}\rangle)_{ll''}^{-1}\langle B_{10}\rangle_{l''l'''}(\langle B_{01}\rangle)_{l'''l'}^{-1} \\ &\quad + O((\ln \varepsilon)^{-3}) \end{aligned} \tag{2.2.53}$$

and (2.2.50) results. ∎

For an explicit determination of the first few of the coefficients $\langle B_{mn}\rangle$ see the next section.

Given Lemmas 2.2.2 and 2.2.4–2.2.7 we are able to state the main result of this section (cf. Theorem 1.2.5 for the corresponding statements if $\gamma = 0$).

Theorem 2.2.8. *Let $y \in \mathbb{R}^3$, $\gamma \in \mathbb{R} - \{0\}$, $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued and assume* (1.2.84). *Then, if $k^2 \in \rho(H_{\gamma,\alpha,y})$ we get $k^2 \in \rho(H_{\gamma,\varepsilon,y})$ for $\varepsilon > 0$ small enough and $H_{\gamma,\varepsilon,y}$ converges to $H_{\gamma,\alpha,y}$ in norm resolvent sense*

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\gamma,\varepsilon,y} - k^2)^{-1} = (H_{\gamma,\alpha,y} - k^2)^{-1},$$

$$k^2 \in \rho(H_{\gamma,\alpha,y}), \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}, \tag{2.2.54}$$

where α is given by

$$\alpha = \begin{cases} \infty & \text{in case I}, \\ \infty & \text{in case II if } \lambda_{01} \neq -|(v, \phi)|^2/4\pi, \\ -[\lambda_{10} + \gamma(\phi, v \ln(|\gamma| x_+/2)v\phi)/4\pi]/|(v, \phi)|^2 & \\ & \text{in case II if } \lambda_{01} = -|(v, \phi)|^2/4\pi, \\ \infty & \text{in case III if } \lambda_{01} \neq 0 \text{ or } \lambda_{01} = 0 \text{ and} \\ & (\tilde{\phi}_l, B_{10}(\gamma, k)\phi_{l'}) \text{ is nonsingular}, \\ \infty & \text{in case IV if } \lambda_{01} \neq -|(v, \phi_1)|^2/4\pi, \\ -[\lambda_{10} + \gamma(\phi_1, v \ln(|\gamma| x_+/2)v\phi_1)/4\pi]/|(v, \phi_1)|^2 & \\ & \text{in case IV if } \lambda_{01} = -|(v, \phi_1)|^2/4\pi. \end{cases} \tag{2.2.55}$$

PROOF. Denoting the limit $\varepsilon \downarrow 0$ of $\varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1}$ by $D_\gamma(k)$ we obtain from the resolvent equation (2.2.21) and from Lemmas 2.2.2 and 2.2.4–2.2.7 that

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\gamma,\varepsilon,y} - k^2)^{-1} = G_{\gamma,k,y} - A_\gamma(k)D_\gamma(k)C_\gamma(k),$$

$$k^2 \in \rho(H_{\gamma,\alpha,y}), \quad \operatorname{Im} k > 0. \tag{2.2.56}$$

The explicit form of $D_\gamma(k)$ and a comparison with (2.1.17) then completes the proof. ∎

At this point remarks similar to that after Theorem 1.2.5 apply. In addition, we would like to mention that the convergence to point interactions can be viewed as a variant of Klauder's phenomenon [292]: In fact, assume $e^{2a|x|}V \in R$ for some $a > 0$ and let V be continuous and monotonously decreasing for $|x| \geq R_0$ for some fixed $R_0 > 0$. Then, in cases II and IV for $\gamma = 0$ and in case II with $\lambda_{01} = -|(v, \phi)|^2/4\pi$ and in case IV with $\lambda_{01} = -|(v, \phi_1)|^2/4\pi$ for $\gamma \neq 0$, we obviously get

$$\lim_{\varepsilon \downarrow 0} \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon)\varepsilon^{-2} V((x - y)/\varepsilon) = 0 \qquad \text{for all } x \neq y \tag{2.2.57}$$

but

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\gamma,\varepsilon,y} - k^2)^{-1} = (H_{\gamma,\alpha,y} - k^2)^{-1} \neq (H_{\gamma,y} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}. \tag{2.2.58}$$

I.2.3 Stationary Scattering Theory

In analogy to Sect. 1.4 we develop scattering theory for Coulomb-plus point interactions and prove that scattering quantities corresponding to $H_{\gamma,\varepsilon,y}$ converge to those of $H_{\gamma,\alpha,y}$ as $\varepsilon \downarrow 0$.

We start with stationary scattering theory for the pair $(H_{\gamma,\alpha,y}, H_{\gamma,y})$. Again we first exploit the rotational symmetry of the problem and mainly treat the case $l = 0$ because of the s-wave nature of the point interaction in $H_{\gamma,\alpha,y}$. The analog of (1.4.1) now reads (cf. (2.2.6))

$$\begin{aligned} \psi_{\gamma,0,\alpha}(k, r) = {} & e^{-\pi\gamma/4k}\Gamma(1 + (i\gamma/2k))\{F_{\gamma,0}^{(0)}(k, r) \\ & + [4\pi\alpha - \gamma F(i\gamma/2k)]^{-1} G_{\gamma,0}^{(0)}(-k, r)\}, \\ & k > 0, \quad -\infty < \alpha \leq \infty, \quad r \geq 0, \quad \gamma \in \mathbb{R}, \end{aligned} \tag{2.3.1}$$

where $F(i\gamma/2k)$ has been defined in (2.1.19). The functions $\psi_{\gamma,0,\alpha}(k, r)$ fulfill (cf. (2.1.9) and (2.1.10))

$$\begin{aligned} & -4\pi\alpha(\psi_{\gamma,0,\alpha}(k))_0 + (\psi_{\gamma,0,\alpha}(k))_1 = 0, \\ & -\psi''_{\gamma,0,\alpha}(k, r) + \gamma r^{-1}\psi_{\gamma,0,\alpha}(k, r) = k^2\psi_{\gamma,0,\alpha}(k, r), \qquad r > 0, \\ & \lim_{\varepsilon \downarrow 0} \lim_{r' \to \infty} e^{-i(k+i\varepsilon)r' + (i\gamma/2k)\ln[2(k+i\varepsilon)r']}[h_{\gamma,0,\alpha} - (k + i\varepsilon)^2]^{-1}(r, r') = \psi_{\gamma,0,\alpha}(k, r), \\ & \qquad r \geq 0; \quad k > 0, \quad -\infty < \alpha \leq \infty, \quad \gamma \in \mathbb{R}. \end{aligned} \tag{2.3.2}$$

Hence $\psi_{\gamma,0,\alpha}(k, r)$ are generalized eigenfunctions of $h_{\gamma,0,\alpha}$. For $l \geq 1$ we obtain (cf. (2.2.6))

$$\begin{aligned} \psi_{\gamma,l}(k, r) = {} & e^{-\pi\gamma/4k}(\Gamma(2l + 2))^{-1}\Gamma(l + 1 + (i\gamma/2k))(2k)^l F_{\gamma,l}^{(0)}(k, r), \\ & k, r > 0, \quad \gamma \in \mathbb{R}, \quad l = 1, 2, \ldots, \end{aligned} \tag{2.3.3}$$

as generalized eigenfunctions associated with $h_{\gamma,l}$, $l = 1, 2, \ldots$. The asymptotic behavior of $\psi_{\gamma,0,\alpha}(k, r)$ as $r \to \infty$ then reads

$$\begin{aligned} \psi_{\gamma,0,\alpha}(k, r) \underset{r \to \infty}{\simeq} {} & k^{-1} e^{i\boldsymbol{\delta}_{\gamma,0,\alpha}(k)} \sin[kr - (\gamma/2k)\ln(2kr) + \boldsymbol{\delta}_{\gamma,0,\alpha}(k)], \\ & k > 0, \quad -\infty < \alpha \leq \infty, \quad \gamma \in \mathbb{R}, \end{aligned} \tag{2.3.4}$$

where the *total phase shift* $\boldsymbol{\delta}_{\gamma,0,\alpha}(k)$ splits up into

$$\boldsymbol{\delta}_{\gamma,0,\alpha}(k) = \delta_{\gamma,0}(k) + \boldsymbol{\delta}^{\text{sc}}_{\gamma,0,\alpha}(k), \qquad k > 0, \quad -\infty < \alpha \leq \infty, \quad \gamma \in \mathbb{R}. \tag{2.3.5}$$

Here

$$\delta_{\gamma,0}(k) = \arg\Gamma(1 + (i\gamma/2k)), \qquad k > 0, \quad \gamma \in \mathbb{R}, \tag{2.3.6}$$

denotes the *pure Coulomb s-wave phase shift* and the *Coulomb modified phase shift* $\boldsymbol{\delta}^{\text{sc}}_{\gamma,0,\alpha}(k)$ is given by

$$e^{2i\boldsymbol{\delta}^{\text{sc}}_{\gamma,0,\alpha}(k)} = 1 + 2\pi i\gamma(e^{\pi\gamma/k} - 1)^{-1}[4\pi\alpha - \gamma F(i\gamma/2k)]^{-1},$$
$$k > 0, \quad -\infty < \alpha \leq \infty, \quad \gamma \in \mathbb{R}. \tag{2.3.7}$$

For $l \geq 1$, we obtain the ordinary Coulomb phase shifts

$$\begin{aligned} &\delta_{\gamma,l}(k) = \arg\Gamma(l + 1 + (i\gamma/2k)), \qquad k > 0, \quad \gamma \in \mathbb{R}, \quad l = 1, 2, \ldots, \\ &\boldsymbol{\delta}^{\text{sc}}_{\gamma,l}(k) \equiv 0, \qquad l = 1, 2, \ldots. \end{aligned} \tag{2.3.8}$$

At this point it is again instructive to compare with the *Coulomb modified effective range expansion* for real-valued spherically symmetric potentials V obeying

$$\int_0^\infty dr\, re^{2ar}|V(r)| < \infty \qquad \text{for some} \quad a > 0. \tag{2.3.9}$$

This low-energy expansion reads (cf., e.g., [95], [96])

$$\begin{aligned} k^{2l}\prod_{m=1}^{l}[1 + (\gamma/2km)^2]\{\pi\gamma(e^{\pi\gamma/k} - 1)^{-1}[\cot\delta^{\text{sc}}_{\gamma,l}(g, k) - i] \\ + \gamma[\Psi(1 + (i\gamma/2k)) - \ln(i|\gamma|/2k) + (ik/\gamma)]\} \\ = -(a^{\text{ac}}_{\gamma,l}(g))^{-1} + 2^{-1}r^{\text{sc}}_{\gamma,l}(g)k^2 + O(k^4), \\ k \geq 0, \quad \gamma, g \in \mathbb{R}, \quad l = 0, 1, \ldots, \end{aligned} \tag{2.3.10}$$

where the right-hand side of (2.3.10) is real analytic in k^2 near $k^2 = 0$ and $\delta^{\text{sc}}_{\gamma,l}(g, k)$ represents the *Coulomb modified phase shift* associated with the Schrödinger operator $-d^2/dr^2 + l(l + 1)/r^2 + \gamma/r \dotplus gV(r)$. In analogy to the short-range case $\gamma = 0$, the coefficients $a^{\text{sc}}_{\gamma,l}(g)$ and $r^{\text{sc}}_{\gamma,l}(g)$, $l = 0, 1, \ldots,$ are called *Coulomb modified partial wave scattering lengths* and *effective range parameters*, respectively.

The fact that

$$\begin{aligned} \pi\gamma(e^{\pi\gamma/k} - 1)^{-1}[\cot\boldsymbol{\delta}^{\text{sc}}_{\gamma,0,\alpha}(k) - i] + \gamma[\Psi(1 + (i\gamma/2k)) - \ln(i|\gamma|/2k) + (ik/\gamma)] \\ = 4\pi\alpha + \gamma[\Psi(1) + \Psi(2)], \end{aligned} \tag{2.3.11}$$

$$\boldsymbol{\delta}^{\text{sc}}_{\gamma,l}(k) \equiv 0, \qquad l = 1, 2, \ldots$$

for the Coulomb-plus point interaction Hamiltonian $H_{\gamma,\alpha,y}$ shows that the Coulomb modified effective range expansion for this interaction is already exact in zeroth order with respect to k^2. In particular, the s-wave Coulomb modified low-energy parameters read

$$\begin{aligned} a^{sc}_{\gamma,0,\alpha} &= -\{4\pi\alpha + \gamma[\Psi(1) + \Psi(2)]\}^{-1}, \\ r^{sc}_{\gamma,0,\alpha} &\equiv 0, \end{aligned} \tag{2.3.12}$$

and all low-energy parameters vanish identically in higher partial waves $l = 1, 2, \ldots$. This proves that the point interaction in $H_{\gamma,\alpha,y}$ is a zero-range as well as s-wave ($l = 0$) interaction.

Next we introduce the scattering wave function associated with $H_{\gamma,\alpha,y}$

$$\Psi_{\gamma,\alpha,y}(k\omega, x) = e^{ik\omega y}\Psi_\gamma(k\omega, x - y) + [4\pi\alpha - \gamma F(i\gamma/2k)]^{-1} \cdot$$
$$\cdot e^{-\pi\gamma/4k}\Gamma(1 + (i\gamma/2k))^2 e^{ik\omega y}|x - y|^{-1}\mathcal{W}_{-i\gamma/2k;\,1/2}(2ie^{-i\pi}k|x - y|),$$
$$k > 0, \quad \omega \in S^2, \quad -\infty < \alpha \le \infty, \quad x, y \in \mathbb{R}^3, \quad x \ne y, \tag{2.3.13}$$

where $\Psi_\gamma(k\omega, x)$ denotes the pure Coulomb scattering wave function

$$\Psi_\gamma(k\omega, x) = e^{-\pi\gamma/4k}\Gamma(1 + (i\gamma/2k))e^{ik\omega x}{}_1F_1((-i\gamma/2k); 1; i(k|x| - k\omega x)),$$
$$k > 0, \quad \omega \in S^2, \quad \gamma \in \mathbb{R}. \tag{2.3.14}$$

A comparison of (2.3.13) with (2.3.1) and (2.3.3) then shows that

$$e^{-ik\omega y}\Psi_{\gamma,\alpha,y}(k\omega, x) = 4\pi|x - y|^{-1}\psi_{\gamma,0,\alpha}(k|x - y|)\overline{Y_{00}(\omega)}\,Y_{00}(\omega_x)$$
$$+ 4\pi|x - y|^{-1}\sum_{l=1}^{\infty}\sum_{m=-l}^{l} i^l\psi_{\gamma,l}(k|x - y|)\overline{Y_{lm}(\omega)}\,Y_{lm}(\omega_x),$$
$$k > 0, \quad -\infty < \alpha \le \infty, \quad \gamma \in \mathbb{R}, \quad x \ne y, \quad \omega_x = x/|x|, \tag{2.3.15}$$

which follows from the well-known partial wave expansion

$$\Psi_\gamma(k\omega, x) = 4\pi|x|^{-1}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l\psi_{\gamma,l}(k, r)\overline{Y_{lm}(\omega)}\,Y_{lm}(\omega_x), \qquad k > 0, \quad \gamma \in \mathbb{R}. \tag{2.3.16}$$

The *Coulomb modified on-shell scattering amplitude* $f^{sc}_{\gamma,\alpha,y}(k, \omega, \omega')$ corresponding to the pair $(H_{\gamma,\alpha,y}, H_{\gamma,y})$ is then defined by

$$f^{sc}_{\gamma,\alpha,y}(k, \omega, \omega') = \lim_{\substack{|x|\to\infty \\ |x|^{-1}x=\omega}} |x|e^{-ik|x| + (i\gamma/2k)\ln(2k|x|)} \cdot$$
$$\cdot [\Psi_{\gamma,\alpha,y}(k\omega', x) - e^{ik\omega' y}\Psi_\gamma(k\omega', x - y)]$$
$$= e^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2[4\pi\alpha - \gamma F(i\gamma/2k)]^{-1}e^{ik(\omega' - \omega)y},$$
$$k > 0, \quad \omega, \omega' \in S^2, \quad \omega \ne \omega', \quad -\infty < \alpha \le \infty, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \tag{2.3.17}$$

The *unitary on-shell scattering operator* $\mathcal{S}_{\gamma,\alpha,y}(k)$ in $L^2(S^2)$ finally reads

$$\mathcal{S}_{\gamma,\alpha,y}(k) = S_{\gamma,y}(k) + 2ike^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2[4\pi\alpha - \gamma F(i\gamma/2k)]^{-1} \cdot$$
$$\cdot (e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00},$$
$$k > 0, \quad -\infty < \alpha \le \infty, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \tag{2.3.18}$$

where ([480], p.198)

$$S_{\gamma,y}(k) = T_y^{-1}(k)[\Gamma(\tfrac{1}{2} + (L^2 + \tfrac{1}{4})^{1/2} - (i\gamma/2k))]^{-1}\Gamma(\tfrac{1}{2} + (L^2 + \tfrac{1}{4})^{1/2} + (i\gamma/2k))T_y(k)$$

$$= T_y^{-1}(k) \bigoplus_{l=0}^{\infty} \bigoplus_{m=-l}^{\infty} \arg \Gamma(l + 1 + (i\gamma/2k))T_y(k),$$

$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \quad (2.3.19)$$

denotes the *pure Coulomb on-shell scattering operator* in $L^2(S^2)$ (with L^2 the square of the angular momentum operator and $(T_y(k)\phi)(\omega) = e^{-ik\omega y}\phi(\omega)$, $\phi \in L^2(S^2)$).

Next we briefly describe stationary scattering theory associated with the Coulomb-type Hamiltonian $H_{\gamma,\varepsilon,y}$. Assume V to be real-valued and

$$e^{2a|\cdot|}V \in R \qquad \text{for some} \quad a > 0 \qquad (2.3.20)$$

for the rest of this section and introduce in $L^2(\mathbb{R}^3)$

$$\Phi^-_{\gamma,\varepsilon,y}(k\omega, x) = u_\varepsilon(x)\Psi_\gamma(k\omega, x),$$

$$\Phi^+_{\gamma,\varepsilon,y}(k\omega, x) = v_\varepsilon(x)\overline{\Psi_\gamma(-k\omega, x)}; \qquad \varepsilon, k > 0, \quad \omega \in S^2, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \quad (2.3.21)$$

where we recall that

$$u_\varepsilon(x) = u((x - y)/\varepsilon), \qquad v_\varepsilon(x) = v((x - y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^3. \quad (2.3.22)$$

The *transition operator* $t_{\gamma,\varepsilon}(k)$ then reads

$$t_{\gamma,\varepsilon}(k) = \varepsilon^{-2}\lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon)[1 + \varepsilon^{-2}\lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon)u_\varepsilon G_{\gamma,k} v_\varepsilon]^{-1},$$

$$0 < \varepsilon < \varepsilon_0, \quad \operatorname{Im} k > -a/\varepsilon_0, \quad k^2 \notin \mathscr{E}_{\gamma,\varepsilon}, \quad \gamma \in \mathbb{R}, \quad (2.3.23)$$

where $\lambda(\cdot, \cdot)$ has been introduced in (2.2.12) and the exceptional set $\mathscr{E}_{\gamma,\varepsilon}$ is given by

$$\mathscr{E}_{\gamma,\varepsilon} = \{k^2 \geq 0 | \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon)uG_{\varepsilon\gamma,\varepsilon k} v\phi_{\gamma,\varepsilon} = -\phi_{\gamma,\varepsilon} \text{ for some}$$

$$\phi_{\gamma,\varepsilon} \in L^2(\mathbb{R}^3), \phi_{\gamma,\varepsilon} \neq 0, k \geqslant 0\}, \qquad \varepsilon > 0, \quad \gamma \in \mathbb{R}. \quad (2.3.24)$$

Due to condition (2.3.20) $\mathscr{E}_{\gamma,\varepsilon}$ is discrete and a compact subset of Lebesgue measure zero [11]. The *Coulomb modified on-shell scattering amplitude* $f^{\mathrm{sc}}_{\gamma,\varepsilon,y}(k, \omega, \omega')$ corresponding to $(H_{\gamma,\varepsilon,y}, H_{\gamma,y})$ is then defined as

$$f^{\mathrm{sc}}_{\gamma,\varepsilon,y}(k, \omega, \omega') = -(4\pi)^{-1}(\Phi^+_{\gamma,\varepsilon,y}(k\omega), t_{\gamma,\varepsilon}(k)\Phi^-_{\gamma,\varepsilon,y}(k\omega')),$$

$$\varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_{\gamma,\varepsilon}, \quad \omega, \omega' \in S^2, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \quad (2.3.25)$$

and the unitary *on-shell scattering operator* $S_{\gamma,\varepsilon,y}(k)$ in $L^2(S^2)$ associated with $H_{\gamma,\varepsilon,y}$ then reads

$$(S_{\gamma,\varepsilon,y}(k)\phi)(\omega) = (S_{\gamma,y}(k)\phi)(\omega) - (k/2\pi i)\int_{S^2} d\omega' f^{\mathrm{sc}}_{\gamma,\varepsilon,y}(k, \omega, \omega')\phi(\omega'),$$

$$\phi \in L^2(S^2), \quad \varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_{\gamma,\varepsilon}, \quad \omega \in S^2, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \quad (2.3.26)$$

Now we are in a position to derive the main results of this section.

Theorem 2.3.1. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued and assume case* I. *Then for $\varepsilon > 0$ small enough*

$$-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega')$$
$$= \varepsilon(v, (1 + uG_0 v)^{-1}u) + O(\varepsilon^2 \ln \varepsilon),$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \quad (2.3.27)$$

PROOF. The expansion (2.3.27) immediately follows from Lemma 2.2.4 and

$$\Psi^{\pm}_{\varepsilon\gamma}(\varepsilon k\omega, x) = e^{-\pi\gamma/4k}\Gamma(1 \pm (i\gamma/2k))\{1 + i\varepsilon k\omega x + [\varepsilon\gamma(|x| \mp \omega x)/2] + O(\varepsilon^2)\},$$
$$\varepsilon \geq 0, \quad k > 0, \quad \gamma \in \mathbb{R}, \quad (2.3.28)$$

since after a translation $x \to x + y$ and a scaling transformation $x \to \varepsilon x$, using (2.2.20), (2.3.25) takes on the form

$$f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega') = -(4\pi)^{-1} e^{-ik(\omega-\omega')y} \lambda(\varepsilon, \gamma\varepsilon \ln \varepsilon) \cdot$$
$$\cdot (u\Psi^{+}_{\varepsilon\gamma}(\varepsilon k\omega), \varepsilon[1 + B_{\gamma,\varepsilon}(k)]^{-1} v\Psi^{-}_{\varepsilon\gamma}(\varepsilon k\omega')). \quad (2.3.29)$$

■

Theorem 2.3.2. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued and assume case* II.

(i) *If $\lambda_{01} = -|(v, \phi)|^2/4\pi$ we get for $\varepsilon > 0$ small enough*

$$-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega')$$
$$= -4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\alpha,y}(k, \omega, \omega')$$
$$+ (\varepsilon\lambda_{10} + (\gamma\varepsilon \ln \varepsilon)\lambda_{01})\langle B_{10}\rangle^{-1}|(v, \phi)|^2 + \varepsilon(v, Tu)$$
$$+ i\varepsilon k\langle B_{10}\rangle^{-1}[(v, \phi)(\phi, \omega' xv) - (\omega xv, \phi)(\phi, v)]$$
$$+ \varepsilon\gamma\langle B_{10}\rangle^{-1}[(v, \phi)(\phi, (|x| - \omega' x)v) + ((|x| + \omega x)v, \phi)(\phi, v)]/2$$
$$- \varepsilon\langle B_{10}\rangle^{-1}[(v, \phi)(\tilde{\phi}, B_{10}Tu) + (v, TB_{10}\phi)(\phi, v)]$$
$$- (\gamma\varepsilon \ln \varepsilon)\langle B_{10}\rangle^{-1}[(v, \phi)(\tilde{\phi}, B_{01}Tu) + (v, TB_{01}\phi)(\phi, v)]$$
$$- \langle B_{10}\rangle^{-2}|(v, \phi)|^2[\varepsilon\langle B_{20}\rangle + (\gamma\varepsilon \ln \varepsilon)\langle B_{11}\rangle + \varepsilon(\gamma \ln \varepsilon)^2\langle B_{02}\rangle]$$
$$+ \langle B_{10}\rangle^{-2}|(v, \phi)|^2\{\varepsilon\langle B_{10}TB_{10}\rangle$$
$$+ (\gamma\varepsilon \ln \varepsilon)\langle[B_{10}TB_{01} + B_{01}TB_{10}]\rangle$$
$$+ \varepsilon(\gamma \ln \varepsilon)^2\langle B_{01}TB_{01}\rangle\} + O(\varepsilon^2(\ln \varepsilon)^3),$$
$$k > 0, \quad \alpha = -\lambda_{10}|(v, \phi)|^{-2}, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \quad (2.3.30)$$

where

$$\langle B_{10}(\gamma, k)\rangle = \lambda_{10} + [\gamma F(i\gamma/2k)|(v, \phi)|^2/4\pi] + [\gamma(\phi, v \ln(|\gamma| x_+/2)v\phi)/4\pi], \quad (2.3.31)$$

$$\langle B_{20}(\gamma, k)\rangle = \lambda_{20} + [\lambda_{10}\gamma F(i\gamma/2k)|(v, \phi)|^2/4\pi]$$

$$
\begin{aligned}
&+ [\lambda_{10}\gamma(\phi, v \ln(|\gamma| x_+/2)v\phi)/4\pi] \\
&+ [\gamma^2 \ln(2k/i|\gamma|)(\phi, v(x_+ + x_-)v\phi)/16\pi] \\
&+ [\gamma^2(\phi, v \ln(|\gamma| x_+/2)(x_+ + x_-)v\phi)/16\pi] \\
&- \Bigg[k^2\{(1 + (i\gamma/2k))(i\gamma/2k)[\Psi(3) - \Psi(1) - \tfrac{1}{2} \\
&- (1 + (i\gamma/2k))^{-1}] - \tfrac{1}{4}\}\left(\phi, v\frac{x_- x_+}{x_+ - x_-}v\phi\right)\Big/ 2\pi\Bigg] \\
&- \Bigg\{k^2\{[-(i\gamma/2k)^2[\Psi(1+(i\gamma/2k)) - \Psi(1) - \Psi(2) + \tfrac{1}{2}]/2] \\
&+ \tfrac{1}{8} + (i\gamma/2k)\}\left(\phi, v\frac{x_-^2}{x_+ - x_-}v\phi\right)\Big/ 2\pi\Bigg\} \\
&- \Bigg\{k^2\{[(i\gamma/2k)^2[\Psi(2 + (i\gamma/2k)) - \Psi(2) - \Psi(3)]/2] \\
&+ (i\gamma/4k)[\Psi(1) - \Psi(3) + (1 + (i\gamma/2k))^{-1}] + \tfrac{1}{8}\}\cdot \\
&\cdot\left(\phi, v\frac{x_+^2}{x_+ - x_-}v\phi\right)\Big/ 2\pi\Bigg\},
\end{aligned}
\tag{2.3.32}
$$

$$
\begin{aligned}
\langle B_{11}(\gamma, k)\rangle = \lambda_{11} &+ [\gamma(\phi, v(x_+ + x_-)v\phi)/16\pi] + [\lambda_{10}|(v, \phi)|^2/4\pi] \\
&+ [\lambda_{01}\gamma(\phi, v \ln(|\gamma| x_+/2)v\phi)/4\pi] \\
&+ [\lambda_{01}\gamma F(i\gamma/2k)|(v, \phi)|^2/4\pi],
\end{aligned}
\tag{2.3.33}
$$

$$
\langle B_{02}\rangle = \lambda_{02} + [\lambda_{01}|(v, \phi)|^2/4\pi], \tag{2.3.34}
$$

and $vH(x_+, x_-)v$ denotes a Hilbert–Schmidt operator with integral kernel

$$
v(x)H(x_+(x, x'), x_-(x, x'))v(x'),
$$
$$
x_\pm(x, x') = |x| + |x'| \pm |x - x'|. \tag{2.3.35}
$$

(ii) *If $\lambda_{01} \neq -|(v, \phi)|^2/4\pi$ we get for $\varepsilon > 0$ small enough*

$$
\begin{aligned}
&-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2}e^{ik(\omega-\omega')y}f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega') \\
&\quad = (\gamma \ln \varepsilon)^{-1}\langle B_{01}\rangle^{-1}|(v, \phi)|^2 - (\gamma \ln \varepsilon)^{-2}\langle B_{01}\rangle^{-2}\langle B_{10}\rangle|(v, \phi)|^2 \\
&\quad + O((\ln \varepsilon)^{-3}), \qquad k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\},
\end{aligned}
\tag{2.3.36}
$$

where

$$
\langle B_{01}\rangle = \lambda_{01} + [|(v, \phi)|^2/4\pi]. \tag{2.3.37}
$$

Proof. Follows directly from Lemma 2.2.5, (2.3.28), and (2.3.29). ■

Theorem 2.3.3. *Let $e^{2a|\cdot|}V \in R$ for some $a > 0$ be real-valued and assume case* III. *If $\lambda_{01} \neq 0$ or $\lambda_{01} = 0$ and $(\tilde{\phi}_l, B_{10}(\gamma, k)\phi_{l'})$, $l, l' = 1, \ldots, N$, is* *nonsingular we get for* $\varepsilon > 0$ *small enough*

$$-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega')$$
$$= \varepsilon(v, Tu) + O((\varepsilon \ln \varepsilon)^2), \qquad k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.38)$$

PROOF. A straightforward consequence of Lemma 2.2.6, (2.3.28), (2.3.29), and $Pu = 0$. ■

Theorem 2.3.4. *Let* $e^{2a|\cdot|}V \in R$ *for some* $a > 0$ *be real-valued and assume case* IV *and* (1.2.84).

(i) *If* $\lambda_{01} = -|(v, \phi_1)|^2/4\pi$ *we get for* $\varepsilon > 0$ *small enough*

$$-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega')$$
$$= -4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\alpha,y}(k, \omega, \omega')$$
$$+ (\lambda_{01}\gamma \ln \varepsilon)^{-1} \langle B_{10}\rangle_{11}^{-2} |(v, \phi_1)|^2 \sum_{l=2}^{N} |\langle B_{10}\rangle_{1l}|^2 + O((\ln \varepsilon)^{-2}),$$
$$k > 0, \quad \alpha = -\lambda_{10}|(v, \phi_1)|^{-2}, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}, \quad (2.3.39)$$

where

$$\langle B_{10}(\gamma, k)\rangle_{11} = \lambda_{10} + [\gamma F(i\gamma/2k)|(v, \phi_1)|^2/4\pi]$$
$$+ [\gamma(\phi_1, v \ln(|\gamma| x_+/2) v\phi_1)/4\pi], \quad (2.3.40)$$
$$\langle B_{10}(\gamma, k)\rangle_{1l} = \gamma(\phi_1, v \ln(|\gamma| x_+/2) v\phi_l)/4\pi, \qquad l = 2, \ldots, N.$$

(ii) *If* $\lambda_{01} \neq -|(v, \phi_1)|^2/4\pi$ *we get for* $\varepsilon > 0$ *small enough*

$$-4\pi e^{\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^{-2} e^{ik(\omega-\omega')y} f^{sc}_{\gamma,\varepsilon,y}(k, \omega, \omega')$$
$$= (\gamma \ln \varepsilon)^{-1} (\langle B_{01}\rangle)_{11}^{-1} |(v, \phi_1)|^2$$
$$- (\gamma \ln \varepsilon)^{-2} |(v, \phi_1)|^2 \sum_{l,l'=1}^{N} (\langle B_{01}\rangle)_{1l}^{-1} \langle B_{10}\rangle_{ll'} (\langle B_{01}\rangle)_{l'1}^{-1}$$
$$+ O((\ln \varepsilon)^{-3}),$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.41)$$

PROOF. Again an immediate consequence of Lemma 2.2.7, (2.3.28), (2.3.29), $(v, \phi_1) \neq 0$, $(v, \phi_l) = 0$, $l = 2, \ldots, N$. ■

By looking at Theorems 2.3.1–2.3.4 one observes that the ω-dependent terms are suppressed by a factor of ε.

Finally, we summarize the corresponding expansion for the on-shell scattering operator $S_{\gamma,\varepsilon,y}(k)$:

Theorem 2.3.5. *Let* $e^{2a|\cdot|}V \in R$ *for some* $a > 0$ *be real-valued and assume* (1.2.84). *Then, for* $\varepsilon > 0$ *small enough, we obtain the norm convergent* *expansions*

$$S_{\gamma,\varepsilon,y}(k) = S_{\gamma,y}(k)$$
$$+ (\varepsilon k/2\pi i)e^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2(v, (1 + uG_0v)^{-1}u)\cdot$$
$$\cdot(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00} + O(\varepsilon^2 \ln \varepsilon) \quad \textit{in case I},$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}. \quad (2.3.42)$$

$$S_{\gamma,\alpha,y}(k) = \mathscr{S}_{\gamma,\alpha,y}(k) + O(\varepsilon(\ln \varepsilon)^2) \quad \textit{in case II if} \quad \lambda_{01} = -|(v, \phi)|^2/4\pi,$$
$$k > 0, \quad \alpha = -\lambda_{10}|(v, \phi)|^{-2}, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R}, \quad (2.3.43)$$

$$S_{\gamma,\varepsilon,y}(k) = S_{\gamma,y}(k)$$
$$+ (\gamma \ln \varepsilon)^{-1}(k/2\pi i)e^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2\langle B_{01}\rangle^{-1}|(v, \phi)|^2\cdot$$
$$\cdot(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00} + O((\ln \varepsilon)^{-2})$$
$$\textit{in case II if} \quad \lambda_{01} \neq -|(v, \phi)|^2/4\pi,$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.44)$$

$$S_{\gamma,\varepsilon,y}(k) = S_{\gamma,y}(k)$$
$$+ (\varepsilon k/2\pi i)e^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2(v, Tu)(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{ik(\cdot)y}Y_{00}$$
$$+ O((\varepsilon \ln \varepsilon)^2) \quad \textit{in case III if } \lambda_{01} \neq 0 \textit{ or } \lambda_{01} = 0 \textit{ and}$$
$$(\tilde{\phi}_l, B_{10}(\gamma, k)\phi_{l'}), \quad l, l' = 1, \ldots, N, \textit{ is nonsingular},$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.45)$$

$$S_{\gamma,\varepsilon,y}(k) = \mathscr{S}_{\gamma,\alpha,y}(k) + O((\ln \varepsilon)^{-1}) \quad \textit{in case IV if} \quad \lambda_{01} = -|(v, \phi_1)|^2/4\pi,$$
$$k > 0, \quad \alpha = -\lambda_{10}|(v, \phi_1)|^{-2}, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.46)$$

$$S_{\gamma,\varepsilon,y}(k) = S_{\gamma,y}(k)$$
$$+ (\gamma \ln \varepsilon)^{-1}(k/2\pi i)e^{-\pi\gamma/2k}\Gamma(1 + (i\gamma/2k))^2(\langle B_{01}\rangle)_{11}^{-1}|(v, \phi_1)|^2\cdot$$
$$\cdot(e^{-ik(\cdot)y}Y_{00}, \cdot)e^{-ik(\cdot)y}Y_{00} + O((\ln \varepsilon)^{-2})$$
$$\textit{in case IV if} \quad \lambda_{01} \neq -|(v, \phi_1)|^2/4\pi,$$
$$k > 0, \quad y \in \mathbb{R}^3, \quad \gamma \in \mathbb{R} - \{0\}. \quad (2.3.47)$$

Again the expansion coefficients in Theorem 2.3.5 become particularly simple by choosing $y = 0$. We also emphasize that only in cases II and IV (i.e., if $H = -\Delta \dot{+} V$ has a zero-energy resonance) if, in addition, $\lambda_{01} = -|(v, \phi)|^2/4\pi$(resp. $\lambda_{01} = -|(v, \phi_1)|^2/4\pi$) the limits $\varepsilon \downarrow 0$ of $f^{\mathrm{sc}}_{\gamma,\varepsilon,y}$ and $S_{\gamma,\varepsilon,y}$ are nontrivial and coincide with $f_{\gamma,\alpha,y}$ and $\mathscr{S}_{\gamma,\alpha,y}$ with α given by (2.2.55). The coefficients $(4\pi)^{-1}(v, (1 + uG_0v)^{-1}u)$ and $(4\pi)^{-1}(v, Tu)$ in $f_{\gamma,\varepsilon,y}$ in cases I and III represent the scattering length of the short-range Hamiltonian $H = -\Delta \dot{+} V$ [11].

As in Sects. 2.1 and 2.2 the above results extend to complex point interactions with Im $\alpha < 0$.

Notes

Section I.2.1

Most of the material of this section is taken from Albeverio, Gesztesy, Høegh-Krohn, and Streit [22]. The operator $h_{\gamma,0,\alpha}$ has first been discussed by Rellich [392] (cf. also Appendix D). In particular, the boundary values ϕ_0, ϕ_1 in (2.1.10) and the determination of $\sigma(h_{\gamma,0,\alpha})$ for $\gamma < 0$ are due to [392]. The resolvent equation (2.1.17) first appeared in Zorbas [512].

Section I.2.2

The estimates needed for the Coulomb Green's function can be found in [96], [99], and [231]. The rest of this section is entirely taken from [22], Sect. 3. Approximations for other long-range + "$\lambda\delta$"-systems appeared in [420].

Section I.2.3

The first part of this section concerning stationary scattering theory for Coulomb plus point interactions extends Sect. 2 in [22]. Stationary scattering theory for Coulomb-type Hamiltonians can be found in [11], [99], and [199]. Theorems 2.3.1–2.3.5 are again taken from [22]. For applications concerning the relation between low-energy parameters for charged and neutral particles, cf. [15], [22], [207], [350]. Applications concerning level shifts in mesic atoms appeared in [22].

CHAPTER I.3

The One-Center δ-Interaction in One Dimension

I.3.1 Basic Properties

There are several ways of introducing the quantum Hamiltonian describing a δ-interaction in one dimension. Following our treatment in Sect. 1.1, we mainly discuss the approach based on self-adjoint extensions of densely defined symmetric operators.

For that purpose we define the closed and nonnegative operator $\dot{H}_y$ in the Hilbert space $L^2(\mathbb{R})$ as

$$\dot{H}_y = -\frac{d^2}{dx^2}, \quad \mathscr{D}(\dot{H}_y) = \{g \in H^{2,2}(\mathbb{R}) | g(y) = 0\} \quad \text{for some} \quad y \in \mathbb{R}, \tag{3.1.1}$$

and note that by the general theory of ordinary differential operators ([158], Ch. XIII.2; [353], Ch. V.17) its adjoint is given by

$$\dot{H}_y^* = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}_y^*) = H^{2,2}(\mathbb{R} - \{y\}) \cap H^{2,1}(\mathbb{R}), \qquad y \in \mathbb{R}, \tag{3.1.2}$$

where $H^{m,n}(\Omega)$ denote corresponding Sobolev spaces. By inspection the equation

$$\dot{H}_y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_y^*), \qquad k^2 \in \mathbb{C} - \mathbb{R}, \qquad \operatorname{Im} k > 0, \tag{3.1.3}$$

has the unique solution

$$\psi(k, x) = e^{ik|x-y|}, \qquad \operatorname{Im} k > 0. \tag{3.1.4}$$

Thus $\dot{H}_y$ has deficiency indices (1, 1) and by Theorem A.1 all self-adjoint extensions $H_{\theta,y}$ of $\dot{H}_y$ are given by the one-parameter family

$$\mathscr{D}(H_{\theta,y}) = \{g + c\psi_+ + ce^{i\theta}\psi_- | g \in \mathscr{D}(\dot{H}_y),\ c \in \mathbb{C}\},$$

$$H_{\theta,y}(g + c\psi_+ + ce^{i\theta}\psi_-) = \dot{H}_y g + ic\psi_+ - ice^{i\theta}\psi_-, \qquad \theta \in [0, 2\pi), \quad y \in \mathbb{R}, \tag{3.1.5}$$

$$\psi_\pm(x) = \frac{i}{2\sqrt{\pm i}} e^{i\sqrt{\pm i}|x-y|}, \qquad \operatorname{Im}\sqrt{\pm i} > 0. \tag{3.1.6}$$

Equations (3.1.5) and (3.1.6) imply $\mathscr{D}(H_{\theta,y}) \subseteq H^{2,1}(\mathbb{R})$. Moreover, a simple calculation using (3.1.1) and (3.1.6) yields (we define $\phi(y\pm) = \lim_{\varepsilon\downarrow 0} \phi(y \pm \varepsilon)$)

$$\begin{aligned}(g + c\psi_+ + ce^{i\theta}\psi_-)'(y+) - (g + c\psi_+ + ce^{i\theta}\psi_-)'(y-) &= -c(1 + e^{i\theta})\\ &= \alpha[g(y) + c\psi_+(y) + ce^{i\theta}\psi_-(y)],\end{aligned} \tag{3.1.7}$$

where we abbreviated

$$\alpha = -2\cos\left(\frac{\theta}{2}\right)\Big/\cos\left(\frac{\theta}{2} - \frac{\pi}{4}\right). \tag{3.1.8}$$

If θ varies in $(0, 2\pi)$, α varies in $\mathbb{R}$ ($\theta \uparrow 2\pi$ corresponds to $\alpha \uparrow +\infty$) and from now on we parametrize all self-adjoint extensions of $\dot{H}_y$ with the help of α. Thus we get

Theorem 3.1.1. *All self-adjoint extensions of $\dot{H}_y$ are given by*

$$-\Delta_{\alpha,y} = -\frac{d^2}{dx^2},$$

$$\mathscr{D}(-\Delta_{\alpha,y}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - \{y\}) | g'(y+) - g'(y-) = \alpha g(y)\},$$
$$-\infty < \alpha \le \infty. \tag{3.1.9}$$

The special case $\alpha = 0$ just leads to the kinetic energy Hamiltonian $-\Delta$ in $L^2(\mathbb{R})$, viz.

$$-\Delta = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}), \tag{3.1.10}$$

whereas the case $\alpha = \infty$ yields a Dirichlet boundary condition at y and hence decouples $(-\infty, y)$ and (y, ∞), viz.

$$\begin{aligned}\mathscr{D}(-\Delta_{\infty,y}) &= \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - \{y\}) | g(y) = 0\}\\ &= H_0^{2,2}((-\infty, y)) \oplus H_0^{2,2}((y, \infty)),\end{aligned} \tag{3.1.11}$$

$$-\Delta_{\infty,y} = (-\Delta_{D-}) \oplus (-\Delta_{D+}), \tag{3.1.12}$$

where $-\Delta_{D\pm}$ denotes the Dirichlet Laplacian on $(y, \pm\infty)$ (see [391], p. 253)

$$\mathscr{D}(-\Delta_{D\pm}) = H_0^{2,2}((y, \pm\infty)). \tag{3.1.13}$$

PROOF. By the arguments sketched above one infers

$$H_{\theta,y} \subseteq -\Delta_{\alpha,y} \tag{3.1.14}$$

with α given by eq. (3.1.8). But $-\Delta_{\alpha,y}$ is easily seen to be symmetric, which completes the proof. ■

By definition $-\Delta_{\alpha,y}$ describes a *δ-interaction of strength α centered at $y \in \mathbb{R}$.* In other words, eq. (3.1.9) is the precise formulation of the formal expression $-d^2/dx^2 + \alpha\delta(x - y)$ used in the physics literature. This is seen as follows: Let formally $V(x) = \alpha\delta(x - y)$ and "integrate" the Schrödinger equation $-\psi''(x) + \alpha\delta(x - y)\psi(x) = E\psi(x)$ from $x = y - \varepsilon$ to $x = y + \varepsilon$ to obtain $-\psi'(y + \varepsilon) + \psi'(y - \varepsilon) + \alpha\psi(y) = E \int_{y-\varepsilon}^{y+\varepsilon} dx\, \psi(x)$. If ε tends to zero we obtain $\psi'(y+) - \psi'(y-) = \alpha\psi(y)$ which is precisely the boundary condition in (3.1.9). A careful physical interpretation of (3.1.9) exhibits characteristic differences to the three-dimensional case (cf. Ch. 1) since now α represents the *coupling constant* of the δ-interaction whereas in three dimensions $-4\pi\alpha$ just describes the inverse *scattering length.*

In the following we summarize basic properties of $-\Delta_{\alpha,y}$:

Theorem 3.1.2. *The resolvent of $-\Delta_{\alpha,y}$ is given by*

$$(-\Delta_{\alpha,y} - k^2)^{-1} = G_k - 2\alpha k(i\alpha + 2k)^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y),$$
$$k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, \quad -\infty < \alpha \le \infty, \quad y \in \mathbb{R}, \tag{3.1.15}$$

with integral kernel

$$(-\Delta_{\alpha,y} - k^2)^{-1}(x, x') = (i/2k)e^{ik|x-x'|} + \alpha(2k)^{-1}(i\alpha + 2k)^{-1}e^{ik[|x-y|+|y-x'|]},$$
$$k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}, \tag{3.1.16}$$

where

$$G_k(x - x') = (i/2k)e^{ik|x-x'|}, \qquad \operatorname{Im} k > 0, \tag{3.1.17}$$

is the integral kernel of $(-\Delta - k^2)^{-1}$ in $L^2(\mathbb{R})$.

PROOF. From (3.1.17) we obtain the general structure of (3.1.15) by (3.1.6) and Theorem A.2. To be more precise, we want to verify Krein's formula (A.4) with $B = -\Delta_{\alpha,y}$, $C = -\Delta$, and $\lambda(k^2) = 2k\alpha/(i\alpha + 2k)$ (we already know that $\phi(k^2, x) = (i/2k)e^{ik|x-y|}$). To this end, let $g \in L^2(\mathbb{R})$ and define

$$h_\alpha(x) = ((-\Delta - k^2)^{-1}g)(x) + \frac{2k\alpha}{i\alpha + 2k}(\phi(k^2), g)\phi(k^2, x) = \frac{i}{2k}\int_{\mathbb{R}} dx'\, e^{ik|x-x'|}g(x')$$
$$+ \frac{\alpha}{2k(i\alpha + 2k)}\int_{\mathbb{R}} dx'\, e^{ik|y-x'|}g(x')e^{ik|x-y|}, \qquad \operatorname{Im} k > 0, \quad k \ne -i\alpha/2. \tag{3.1.18}$$

Clearly, $h_\alpha \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - \{y\})$ and by a straightforward computation

$$h_\alpha'(y+) - h_\alpha'(y-) = \frac{i\alpha}{(i\alpha + 2k)}\int_{\mathbb{R}} dx'\, e^{ik|y-x'|}g(x') = \alpha h_\alpha(y). \tag{3.1.19}$$

Equation (3.1.19) then implies that $h_\alpha \in \mathscr{D}(-\Delta_{\alpha,y})$ and from

$$((-\Delta_{\alpha,y} - k^2)h_\alpha)(x) = -h_\alpha''(x) - k^2 h_\alpha(x) = g(x), \qquad x \in \mathbb{R} - \{y\}, \tag{3.1.20}$$

we obtain (3.1.15). ■

As in the three-dimensional case we add additional domain properties of $-\Delta_{\alpha,y}$ and point out the locality of the one-center δ-interaction:

Theorem 3.1.3. *The domain $\mathscr{D}(-\Delta_{\alpha,y})$, $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}$, consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) - 2k\alpha(i\alpha + 2k)^{-1}\phi_k(y)G_k(x - y), \tag{3.1.21}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ and $k^2 \in \rho(-\Delta_{\alpha,y})$, $\operatorname{Im} k > 0$. The decomposition (3.1.21) is unique and with $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ of this form we obtain

$$(-\Delta_{\alpha,y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{3.1.22}$$

Next, let $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ and suppose that $\psi = 0$ in an open set $U \subseteq \mathbb{R}$. Then $-\Delta_{\alpha,y}\psi = 0$ in U.

PROOF. Since the proof is analogous to that of Theorem 1.1.3 we omit the details. ■

Finally, we discuss spectral properties of $-\Delta_{\alpha,y}$:

Theorem 3.1.4. *Let $-\infty < \alpha \leq \infty$, $y \in \mathbb{R}$. Then the essential spectrum of $-\Delta_{\alpha,y}$ is purely absolutely continuous and covers the nonnegative real axis*

$$\sigma_{\mathrm{ess}}(-\Delta_{\alpha,y}) = \sigma_{\mathrm{ac}}(-\Delta_{\alpha,y}) = [0, \infty), \qquad \sigma_{\mathrm{sc}}(-\Delta_{\alpha,y}) = \varnothing. \tag{3.1.23}$$

If $-\infty < \alpha < 0$, $-\Delta_{\alpha,y}$ has precisely one negative, simple eigenvalue, i.e., its point spectrum $\sigma_p(-\Delta_{\alpha,y})$ reads

$$\sigma_p(-\Delta_{\alpha,y}) = \{-\alpha^2/4\}, \qquad -\infty < \alpha < 0, \tag{3.1.24}$$

with

$$(-\alpha/2)^{1/2}e^{\alpha|x-y|/2}, \qquad -\infty < \alpha < 0, \tag{3.1.25}$$

its strictly positive (normalized) eigenfunction. If $\alpha \geq 0$ or $\alpha = +\infty$, $-\Delta_{\alpha,y}$ has no eigenvalues,

$$\sigma_p(-\Delta_{\alpha,y}) = \varnothing, \qquad \alpha \notin (-\infty, 0). \tag{3.1.26}$$

PROOF. Since one can follow the proof of Theorem 1.1.4 step by step we omit any details. ■

The pole structure $(i\alpha + 2k)^{-1}$ of (3.1.16) with respect to k not only determines the point spectrum but also gives the existence of resonances for the δ-interaction Hamiltonian $-\Delta_{\alpha,y}$: If $\alpha \geq 0$, then $-\Delta_{\alpha,y}$ has a simple resonance at $k_0 = -i\alpha/2$ with corresponding resonance function $\psi_{k_0}(x) = e^{\alpha|x-y|/2}$, $\alpha \geq 0$

(note that for $\alpha \neq 0$ the apparent first-order pole at $k = 0$ actually cancels in (3.1.16)).

An alternative way of introducing δ-interactions of strength α centered at y can be obtained from the theory of quadratic forms. The form $Q_{\alpha,y}$ in $L^2(\mathbb{R})$ defined as

$$Q_{\alpha,y}(g, h) = (g', h') + \alpha\overline{g(y)}h(y), \qquad \mathscr{D}(Q_{\alpha,y}) = H^{2,1}(\mathbb{R}), \quad \alpha, y \in \mathbb{R}, \quad (3.1.27)$$

is easily seen to be densely defined, semibounded, and closed. The unique self-adjoint operator associated with $Q_{\alpha,y}$ is just given by $-\Delta_{\alpha,y}$ (see, e.g., [389], p. 168, [41], [188], [510], [511], [512]). Note that this approach does not work in three dimensions since there is no appropriate closable form in this case. Another possibility of defining δ-interactions is provided by the use of *local Dirichlet forms* as developed in [32], [33] (cf. Appendix F): Consider in $L^2(\mathbb{R}; \phi_{\alpha,y}^2\, dx)$ the energy form

$$\dot{E}_{\alpha,y}(g, h) = \int_{\mathbb{R}} dx\, \phi_{\alpha,y}^2(x)\overline{g'(x)}h'(x), \qquad \mathscr{D}(\dot{E}_{\alpha,y}) = C_0^1(\mathbb{R}), \quad (3.1.28)$$

where

$$\phi_{\alpha,y}(x) = e^{\alpha|x-y|/2}, \qquad \alpha, y \in \mathbb{R}. \quad (3.1.29)$$

It follows that $\dot{E}_{\alpha,y}$ is closable and that $\phi_{\alpha,y}^{-1}(-\Delta_{\alpha,y} + (\alpha^2/4))\phi_{\alpha,y}$ is the unique self-adjoint operator associated with its closure. As shown in Sect. 1.1 and Appendix F this method is also applicable in the three- and two-dimensional cases.

We finally note that the above results are not confined to self-adjoint extensions ($\alpha \in \mathbb{R}$) of $\dot{H}_y$, but easily generalize to accretive extensions of $i\dot{H}_y$ ($\operatorname{Im} \alpha < 0$) and thus to complex δ-interactions.

I.3.2 Approximations by Means of Local Scaled Short-Range Interactions

In this section we show how to approximate $-\Delta_{\alpha,y}$ by means of scaled short-range Hamiltonians in the norm resolvent sense. We first introduce some notations. Let

$$G_k = (-\Delta - k^2)^{-1}, \qquad \operatorname{Im} k > 0, \quad (3.2.1)$$

$$G_k(x, x') = \frac{i}{2k} e^{ik|x-x'|}, \qquad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}, \quad (3.2.2)$$

denote the "free" resolvent and its integral kernel. If $V \in L^1(\mathbb{R})$ is real-valued (which we assume from now on) we define

$$v(x) = |V(x)|^{1/2}, \qquad u(x) = |V(x)|^{1/2} \operatorname{sgn}[V(x)] \quad (3.2.3)$$

such that $uv = V$. Then we note

Lemma 3.2.1. *Let $V \in L^1(\mathbb{R})$. Then V is form compact with respect to $-\Delta$, i.e.,*

$$|V|^{1/2}(-\Delta + E)^{-1/2} \in \mathscr{B}_\infty(L^2(\mathbb{R})), \qquad E > 0. \tag{3.2.4}$$

In particular,

$$uG_k v \in \mathscr{B}_2(L^2(\mathbb{R})), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0, \tag{3.2.5}$$

and

$$uG_k v \in \mathscr{B}_1(L^2(\mathbb{R})), \qquad \operatorname{Im} k > 0. \tag{3.2.6}$$

If, in addition, $(1 + |\cdot|)^{1+\delta} V \in L^1(\mathbb{R})$ for some $\delta > 0$, then

$$uG_k v \in \mathscr{B}_1(L^2(\mathbb{R})), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0. \tag{3.2.7}$$

Proof. Equations (3.2.4) and (3.2.5) follow from

$$\frac{1}{4|k|^2} \int_{\mathbb{R}^2} dx\, dx' |V(x)| e^{-2 \operatorname{Im} k |x - x'|} |V(x')| < \infty, \qquad \operatorname{Im} k \geq 0, \quad k \neq 0. \tag{3.2.8}$$

Equation (3.2.6) is discussed in [391], p. 384, and (3.2.7) is proved in [438], p. 72. ∎

Next we introduce

$$\tilde{v}(x) = v(x - \varepsilon^{-1} y), \qquad \tilde{u}(x) = u(x - \varepsilon^{-1} y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}, \tag{3.2.9}$$

and

$$\tilde{B}(\varepsilon, k) = \lambda(\varepsilon) \tilde{u} G_k \tilde{v}, \qquad \operatorname{Im} k > 0, \tag{3.2.10}$$

where λ is real-analytic near the origin with $\lambda(0) = 0$. By the estimate (3.2.8), $\tilde{B}(\varepsilon, k)$ extends to a Hilbert–Schmidt operator for $\operatorname{Im} k \geq 0$, $k \neq 0$, and due to (3.2.4) the form sum

$$H_y(\varepsilon) = -\Delta \dotplus \lambda(\varepsilon) V(\cdot - \varepsilon^{-1} y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}, \tag{3.2.11}$$

is well defined (cf. Appendix B). Moreover, from Theorem B.1(b) we infer the resolvent equation

$$(H_y(\varepsilon) - k^2)^{-1} = G_k - \lambda(\varepsilon) G_k \tilde{v} [1 + \tilde{B}(\varepsilon, k)]^{-1} \tilde{u} G_k,$$
$$k^2 \in \rho(H_y(\varepsilon)), \quad \operatorname{Im} k > 0. \tag{3.2.12}$$

In addition, we introduce the unitary scaling group

$$(U_\varepsilon g)(x) = \varepsilon^{-1/2} g(x/\varepsilon), \qquad \varepsilon > 0, \quad g \in L^2(\mathbb{R}), \tag{3.2.13}$$

and the family $H_{\varepsilon, y}$ of self-adjoint operators

$$H_{\varepsilon, y} = \varepsilon^{-2} U_\varepsilon H_y(\varepsilon) U_\varepsilon^{-1} = -\Delta \dotplus \lambda(\varepsilon) \varepsilon^{-2} V((\cdot - y)/\varepsilon),$$
$$\varepsilon > 0, \quad y \in \mathbb{R}. \tag{3.2.14}$$

In order to discuss the limit of $H_{\varepsilon, y}$ as $\varepsilon \downarrow 0$ it is convenient to define Hilbert–

Schmidt operators $A_\varepsilon(k)$, $B_\varepsilon(k)$, $C_\varepsilon(k)$, $\varepsilon > 0$, with integral kernels

$$A_\varepsilon(k, x, x') = G_k(x - y - \varepsilon x')v(x'), \qquad \operatorname{Im} k > 0, \tag{3.2.15}$$

$$B_\varepsilon(k, x, x') = \varepsilon^{-1}\lambda(\varepsilon)u(x)G_k(\varepsilon(x - x'))v(x'), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0, \tag{3.2.16}$$

$$C_\varepsilon(k, x, x') = u(x)G_k(\varepsilon x + y - x'), \qquad \operatorname{Im} k > 0. \tag{3.2.17}$$

Then a translation $x \to x + (y/\varepsilon)$, $\varepsilon > 0$, together with

$$\varepsilon^2 U_\varepsilon G_k U_\varepsilon^{-1} = G_{k/\varepsilon} \tag{3.2.18}$$

leads to

$$\begin{aligned}(H_{\varepsilon,y} - k^2)^{-1} &= \varepsilon^2 U_\varepsilon[H_y(\varepsilon) - (\varepsilon k)^2]^{-1} U_\varepsilon^{-1} \\ &= G_k - \varepsilon^{-1}\lambda(\varepsilon)A_\varepsilon(k)[1 + B_\varepsilon(k)]^{-1}C_\varepsilon(k), \\ &\qquad \varepsilon > 0, \quad k^2 \in \rho(H_{\varepsilon,y}), \quad \operatorname{Im} k > 0, \quad y \in \mathbb{R}. \end{aligned} \tag{3.2.19}$$

Convergence properties of A_ε, B_ε, and C_ε are summarized in

Lemma 3.2.2. *Define rank-one operators $A(k)$, $B(k)$, $C(k)$, through their integral kernels*

$$A(k, x, x') = G_k(x - y)v(x'), \qquad \operatorname{Im} k > 0, \tag{3.2.20}$$

$$B(k, x, x') = \lambda'(0)G_k(0)u(x)v(x'), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0, \tag{3.2.21}$$

$$C(k, x, x') = u(x)G_k(y - x'), \qquad \operatorname{Im} k > 0. \tag{3.2.22}$$

Then, for fixed k, $\operatorname{Im} k > 0$, $A_\varepsilon(k)$, $B_\varepsilon(k)$, $C_\varepsilon(k)$ converge in Hilbert–Schmidt norm to $A(k)$, $B(k)$, $C(k)$, respectively, as $\varepsilon \downarrow 0$.

PROOF. Clearly,

$$\operatorname*{w-lim}_{\varepsilon\downarrow 0} A_\varepsilon(k) = A(k), \qquad \operatorname*{w-lim}_{\varepsilon\downarrow 0} B_\varepsilon(k) = B(k), \qquad \operatorname*{w-lim}_{\varepsilon\downarrow 0} C_\varepsilon(k) = C(k) \tag{3.2.23}$$

by dominated convergence. By Theorem 2.21 of [438] it suffices to prove

$$\lim_{\varepsilon\downarrow 0} \|A_\varepsilon(k)\|_2 = \|A(k)\|_2, \qquad \lim_{\varepsilon\downarrow 0} \|B_\varepsilon(k)\|_2 = \|B(k)\|_2, \qquad \lim_{\varepsilon\downarrow 0} \|C_\varepsilon(k)\|_2 = \|C(k)\|_2, \tag{3.2.24}$$

which is obviously true. ∎

Now we are prepared for the main result of this section and state

Theorem 3.2.3. *Suppose $V \in L^1(\mathbb{R})$ is real-valued and $y \in \mathbb{R}$. Then, if $k^2 \in \rho(-\Delta_{\alpha,y})$, we get $k^2 \in \rho(H_{\varepsilon,y})$ for $\varepsilon > 0$ small enough and $H_{\varepsilon,y}$ converges to $-\Delta_{\alpha,y}$ in norm resolvent sense*

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}, \qquad y \in \mathbb{R}, \tag{3.2.25}$$

where

$$\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x). \tag{3.2.26}$$

PROOF. From (3.2.19) and Lemma 3.2.2 we conclude

$$\underset{\varepsilon \downarrow 0}{\text{n-lim}}\, (H_{\varepsilon,y} - k^2)^{-1} = G_k - \lambda'(0)A(k)[1 + B(k)]^{-1}C(k),$$

$$k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0. \tag{3.2.27}$$

Now

$$B(k) = \lambda'(0)G_k(0)(v, \cdot)u \tag{3.2.28}$$

implies

$$[1 + B(k)]^{-1} = 1 - \lambda'(0)G_k(0)[1 + \lambda'(0)(v, u)G_k(0)]^{-1}(v, \cdot)u, \tag{3.2.29}$$

and insertion of (3.2.29) into (3.2.27) gives (3.1.15) with $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x)$. ■

In particular, $H_{\varepsilon,y}$ converges to $-\Delta$ as $\varepsilon \downarrow 0$ if and only if $\lambda'(0)\int_{\mathbb{R}} dx\, V(x) = 0$, i.e., if the δ-interation at the point y has vanishing strength. We would like to emphasize that this kind of approximation scheme automatically yields interactions with finite strength, $|\alpha| < \infty$. The case $\alpha = +\infty$, corresponding to a Dirichlet boundary condition which completely separates $\mathbb{R}$ into $(-\infty, y)$ and (y, ∞), is thereby excluded.

In contrast to the three-dimensional case no zero-energy properties of $H = -\Delta \dotplus V$ enter into the above discussion.

We now note that Theorem 3.2.3 has a simple interpretation in terms of "δ-sequences": For smooth functions V the potential term in $H_{\varepsilon,y}$ may be written as

$$[\lambda'(0) + O(\varepsilon)]\frac{1}{\varepsilon}V\left(\frac{1}{\varepsilon}(x - y)\right), \tag{3.2.30}$$

which converges to $[\lambda'(0)\int_{\mathbb{R}} dx'\, V(x')]\delta(x - y)$ in the sense of distributions ([197], Ch. I.2]) as $\varepsilon \downarrow 0$.

Of course, $\lambda(\varepsilon)$ need not be real-valued. The proof of Theorem 3.2.3 extends in a straightforward manner to the case of complex δ-interactions (cf. the end of Sect. 3.1). We also remark that the above proof indicates another possibility of defining bound states or resonances of $-\Delta_{\alpha,y}$ in terms of (simple) zeros of the Fredholm determinant

$$\det[1 + B(k)] = 1 + \operatorname{Tr}[B(k)] = 1 + \frac{i}{2k}\lambda'(0)\int_{\mathbb{R}} dx\, V(x) = 1 + (i\alpha/2k) \tag{3.2.31}$$

(note that by (3.2.28) $B(k)$ is of rank one).

Consequences of Theorem 3.2.3 concerning convergence of eigenvalues and resonances and convergence of the scattering matrix are discussed in the following two sections. Here we only note that (3.2.25) implies strong convergence of the evolution groups $e^{-itH_{\varepsilon,y}}$ to $e^{-it(-\Delta_{\alpha,y})}$ uniformly with respect to t for t varying in compact intervals ([283], p. 504) as $\varepsilon \downarrow 0$.

I.3.3 Convergence of Eigenvalues and Resonances

In this section we go one step further and prove convergence of eigenvalues and resonances of $H_{\varepsilon,y}$ towards that of $-\Delta_{\alpha,y}$ as $\varepsilon \downarrow 0$. First, we note that Theorem B.1(b) applied to $H_y(\varepsilon)$ and $H_{\varepsilon,y}$ immediately yields

$$\sigma_{\text{ess}}(H_{\varepsilon,y}) = \sigma_{\text{ess}}(H_y(\varepsilon)) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad \varepsilon > 0, \quad y \in \mathbb{R}. \tag{3.3.1}$$

By Theorem 3.1.4 the same results hold in the limit $\varepsilon \downarrow 0$,

$$\sigma_{\text{ess}}(-\Delta_{\alpha,y}) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}. \tag{3.3.2}$$

Having located the essential spectrum we now turn to a discussion of the discrete spectrum.

A detailed analysis of $B_\varepsilon(k)$ yields

Theorem 3.3.1. *Assume $e^{2a|\cdot|}V \in L^1(\mathbb{R})$ for some $a > 0$ is real-valued and let $y \in \mathbb{R}$.*

(a) *If $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ with $\alpha < 0$, $-\Delta_{\alpha,y}$ has the simple eigenvalue $E_0 = k_0^2 < 0$, $k_0 = -i\alpha/2 = -(i/2)\lambda'(0)\int_{\mathbb{R}} dx\, V(x)$ and for $\varepsilon > 0$ small enough, $\sigma(H_{\varepsilon,y}) \cap (-\infty, 0)$ consists precisely of one simple eigenvalue $E_\varepsilon = k_\varepsilon^2 < 0$ which is analytic in ε near $\varepsilon = 0$*

$$\begin{aligned} k_\varepsilon = i\sqrt{-E_\varepsilon} &= k_0 - \frac{i}{4}\lambda''(0)\varepsilon \int_{\mathbb{R}} dx\, V(x) \\ &\quad - \frac{i}{4}\lambda'(0)^2\varepsilon \int_{\mathbb{R}^2} dx\, dx'\, V(x)|x - x'|V(x') + O(\varepsilon^2). \end{aligned} \tag{3.3.3}$$

(b) *If $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,y})$ with $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x) > 0$, $-\Delta_{\alpha,y}$ has no eigenvalues and for $\varepsilon > 0$ small enough $H_{\varepsilon,y}$ also has no negative eigenvalues.*

(c) *If $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = G_k$, $k^2 \in \rho(-\Delta)$, or equivalently, if $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x) = 0$, then as $\varepsilon \downarrow 0$, $H_{\varepsilon,y}$ has at most one negative eigenvalue $E_\varepsilon = k_\varepsilon^2 < 0$ analytic in ε near $\varepsilon = 0$ which is absorbed into the essential spectrum*

$$\begin{aligned} k_\varepsilon = i\sqrt{-E_\varepsilon} &= -\frac{i}{4}\lambda''(0)\varepsilon \int_{\mathbb{R}} dx\, V(x) \\ &\quad - \frac{i}{4}\lambda'(0)^2\varepsilon \int_{\mathbb{R}^2} dx\, dx'\, V(x)|x - x'|V(x') + O(\varepsilon^2). \end{aligned} \tag{3.3.4}$$

PROOF. We first note that due to (3.2.19) and Theorem B.1(c), $H_{\varepsilon,y}$ has an eigenvalue $E_\varepsilon = k_\varepsilon^2 < 0$ if and only if $B_\varepsilon(k)$ has an eigenvalue -1, i.e., if

$$B_\varepsilon(k_\varepsilon)\phi_\varepsilon = -\phi_\varepsilon, \qquad \phi_\varepsilon \in L^2(\mathbb{R}), \quad \phi_\varepsilon \neq 0, \quad \varepsilon > 0, \tag{3.3.5}$$

and also the corresponding (geometric) multiplicity remains preserved.

Next, following [435], we decompose

$$B_\varepsilon(k) = L_\varepsilon(k) + M_\varepsilon(k), \qquad k \neq 0, \quad \mathrm{Im}\, k > -a/\varepsilon_0, \quad 0 \le \varepsilon < \varepsilon_0, \tag{3.3.6}$$

with

$$L_\varepsilon(k, x, x') = \frac{i}{2k}\varepsilon^{-1}\lambda(\varepsilon)u(x)v(x'), \qquad k \in \mathbb{C} - \{0\}, \tag{3.3.7}$$

$$M_\varepsilon(k, x, x') = \frac{i}{2k}\varepsilon^{-1}\lambda(\varepsilon)u(x)[e^{i\varepsilon k|x-x'|} - 1]v(x'), \qquad \mathrm{Im}\, k > -a/\varepsilon_0. \tag{3.3.8}$$

Obviously, $M_\varepsilon(k)$ is analytic in (ε, k) for $|\varepsilon|$ small and $\mathrm{Im}\, k > -a/\varepsilon_0$, and one infers the (norm convergent) expansion

$$M_\varepsilon(k) = \varepsilon N + O(\varepsilon^2), \qquad \mathrm{Im}\, k > -a/\varepsilon_0, \tag{3.3.9}$$

$$N(x, x') = -\tfrac{1}{2}\lambda'(0)u(x)|x - x'|v(x') \tag{3.3.10}$$

uniformly in k if k varies in compact subsets of $\mathrm{Im}\, k > -a/\varepsilon_0$. Equation (3.3.9) and the formula ([438], p. 49)

$$\det(1 + A + B + AB) = \det(1 + A)\det(1 + B) \tag{3.3.11}$$

imply

$$\det[1 + B_\varepsilon(k)] = \det[1 + M_\varepsilon(k)]\det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}. \tag{3.3.12}$$

One then concludes that $k^2 < 0$ is an eigenvalue of $H_{\varepsilon,y}$ if and only if

$$\begin{aligned}\det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\} &= 1 + \mathrm{Tr}\{[1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}\\ &= 1 + \frac{i}{2k}\varepsilon^{-1}\lambda(\varepsilon)(u, [1 + M_\varepsilon(k)]^{-1}v) = 0.\end{aligned} \tag{3.3.13}$$

Since $[1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)$ has rank one and is analytic in ε and k for $|\varepsilon|$ small and $\mathrm{Im}\, k > -a/\varepsilon_0$, $k \neq 0$, $\det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}$ is analytic with respect to ε and k in the same domain [261]. The fact that k_0 is a simple zero of the Fredholm determinant

$$\det[1 + L_0(k)] = 1 + \frac{i}{2k}\lambda'(0)\int_{\mathbb{R}} dx\, V(x) \tag{3.3.14}$$

and

$$\det[1 + L_0(k_0)] = 0, \qquad \frac{\partial}{\partial k}\det[1 + L_0(k)]|_{k=k_0} \neq 0 \tag{3.3.15}$$

proves by the implicit function theorem that in a neighborhood of $(0, k_0)$, $\det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}$ has precisely one simple zero k_ε which is analytic in ε near $\varepsilon = 0$

$$k_\varepsilon = k_0 + O(\varepsilon). \tag{3.3.16}$$

By Theorems B.1(c) and B.2, $E_\varepsilon = k_\varepsilon^2 < 0$ is a simple eigenvalue of $H_{\varepsilon,y}$. Inserting

$$[1 + M_\varepsilon(k)]^{-1} = 1 - \varepsilon N - [M_\varepsilon(k) - \varepsilon N] + M_\varepsilon(k)^2[1 + M_\varepsilon(k)]^{-1} \tag{3.3.17}$$

into (3.3.13), solving for k as a function of ε yields (3.3.3). Since any solution k_ε of (3.3.13) obeys (3.3.16) part (a) is proved.

If $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\; V(x) > 0$ then, for ε small enough, any solution k_ε of (3.3.13) has $\operatorname{Im} k_\varepsilon < 0$ which proves part (b).

To prove (c) we multiply $\det[1 + L_0(k)]$ and $\det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}$ by k. Then

$$\{k \det[1 + L_0(k)]\}|_{k=0} = 0, \qquad \frac{\partial}{\partial k}\{k \det[1 + L_0(k)]\} = 1 \tag{3.3.18}$$

and analyticity of $k \det\{1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}$ near $\varepsilon = k = 0$ again proves by the implicit function theorem that in a neighborhood of $\varepsilon = k = 0$, $k \det\{(1 + [1 + M_\varepsilon(k)]^{-1}L_\varepsilon(k)\}$ has one simple zero k_ε which is analytic in ε

$$k_\varepsilon = \varepsilon k_1 + O(\varepsilon^2) \tag{3.3.19}$$

and k_ε^2 is a negative eigenvalue of $H_{\varepsilon,y}$ iff $\operatorname{Im} k_\varepsilon > 0$ for $\varepsilon > 0$. The rest follows from the proof of part (a). ∎

If, e.g., in Theorem 3.3.1(c) $\lambda'(0) \neq 0$, $\int_{\mathbb{R}} dx\; V(x) = 0$, or if $\lambda'(0) = 0$, $\int_{\mathbb{R}} dx\; V(x) \neq 0, \lambda''(0) \neq 0$, then $k_1 \neq 0$ in (3.3.19) ($\int_{\mathbb{R}^2} dx\, dx'\; V(x)|x - x'|\, V(x')$ is strictly negative if $\int_{\mathbb{R}} dx\; V(x) = 0$ [435]).

Theorem 3.3.1(a) and (c) describe the convergence of eigenvalues of $H_{\varepsilon,y}$ to those of $-\Delta_{\alpha,y}$. For *resonances* (contained in Theorem 3.3.1(b)) the corresponding result reads

Theorem 3.3.2. *Let $y \in \mathbb{R}$ and assume that $e^{2a|\cdot|}V \in L^1(\mathbb{R})$ for all $a > 0$ is real-valued. If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}$ *with* $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\; V(x) > 0$, *then $-\Delta_{\alpha,y}$ has the simple resonance $k_0 = -i\alpha/2 = -(i/2)\lambda'(0)\int_{\mathbb{R}} dx\; V(x)$ and, for $\varepsilon > 0$ small enough, $H_{\varepsilon,y}$ has precisely one simple resonance k_ε,* $\operatorname{Im} k_\varepsilon < 0$, *near k_0 which is analytic in ε near $\varepsilon = 0$ and fulfills* (3.3.3). *Similarly, if $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\; V(x) = 0$, then, for $\varepsilon > 0$ small enough, $H_{\varepsilon,y}$ has at most one simple resonance k_ε which is analytic in ε near $\varepsilon = 0$ and fulfills* (3.3.4).

PROOF. Starting with (3.3.6) the proof is identical to that of Theorem 3.3.1(a) and (c) with the only exception that now $\operatorname{Im} k_\varepsilon < 0$. ∎

In sharp contrast to the corresponding three-dimensional results in Sect. 1.3 zero-energy properties of $H = -\Delta \dotplus V$ played no role in Theorems 3.3.1–3.3.3. In addition, there are no eigenvalues of $H_{\varepsilon,y}$ approaching infinity as $\varepsilon \downarrow 0$.

I.3.4 Stationary Scattering Theory

Finally, we develop scattering theory for δ-interactions and prove convergence of the scattering matrix associated with $H_{\varepsilon,y}$ to that of the δ-interaction Hamiltonian $-\Delta_{\alpha,y}$ as $\varepsilon \downarrow 0$.

We start with the scattering wave functions of $-\Delta_{\alpha,y}$. Define

$$\Psi_{\alpha,y}(k, \sigma, x) = e^{ik\sigma x} - i\alpha(2k + i\alpha)^{-1}e^{ik\sigma y}e^{ik|x-y|},$$
$$k \geq 0, \quad \sigma = \pm 1, \quad -\infty < \alpha \leq \infty, \quad x, y \in \mathbb{R}. \tag{3.4.1}$$

Then by inspection

$$\begin{aligned}
&\Psi_{\alpha,y}(k,\sigma,y+) = \Psi_{\alpha,y}(k,\sigma,y-),\\
&\Psi'_{\alpha,y}(k,\sigma,y+) - \Psi'_{\alpha,y}(k,\sigma,y-) = \alpha\Psi_{\alpha,y}(k,\sigma,y),\\
&-\Psi''_{\alpha,y}(k,\sigma,x) = k^2\Psi_{\alpha,y}(k,\sigma,x), \qquad x \in \mathbb{R} - \{y\},\\
&\lim_{\varepsilon\downarrow 0}\lim_{x'\to\mp\infty} (2k/i)e^{\pm i(k+i\varepsilon)x'}[-\Delta_{\alpha,y} - (k+i\varepsilon)^2]^{-1}(x,x') = \Psi_{\alpha,y}(k,\pm 1,x),\\
&\qquad\qquad x \in \mathbb{R};\quad k \geq 0,
\end{aligned} \tag{3.4.2}$$

which shows that $\Psi_{\alpha,y}(k,\sigma)$ are generalized eigenfunctions ([353], Ch. VI) associated with $-\Delta_{\alpha,y}$ corresponding to left ($\sigma = +1$) and right ($\sigma = -1$) incidence. The corresponding *transmission* and *reflection coefficients* from the left and right are then defined by

$$\begin{aligned}
\mathcal{T}^{\mathrm{l}}_{\alpha,y}(k) &= \lim_{x\to+\infty} e^{-ikx}\Psi_{\alpha,y}(k,+1,x),\\
\mathcal{T}^{\mathrm{r}}_{\alpha,y}(k) &= \lim_{x\to-\infty} e^{+ikx}\Psi_{\alpha,y}(k,-1,x),\\
\mathcal{R}^{\mathrm{l}}_{\alpha,y}(k) &= \lim_{x\to-\infty} e^{+ikx}[\Psi_{\alpha,y}(k,+1,x) - e^{ikx}],\\
\mathcal{R}^{\mathrm{r}}_{\alpha,y}(k) &= \lim_{x\to+\infty} e^{-ikx}[\Psi_{\alpha,y}(k,-1,x) - e^{-ikx}],
\end{aligned} \tag{3.4.3}$$

where $\mathcal{T}^{\mathrm{l}}_{\alpha,y}(k)$ equals $\mathcal{T}^{\mathrm{r}}_{\alpha,y}(k)$ because of time reversal invariance. Explicitly, we get

$$\mathcal{T}^{\mathrm{l}}_{\alpha,y}(k) = (2k+i\alpha)^{-1}2k = \mathcal{T}^{\mathrm{r}}_{\alpha,y}(k), \tag{3.4.4}$$

$$\mathcal{R}^{\mathrm{l}}_{\alpha,y}(k) = -(2k+i\alpha)^{-1}i\alpha e^{2iky}, \tag{3.4.5}$$

$$\mathcal{R}^{\mathrm{r}}_{\alpha,y}(k) = -(2k+i\alpha)^{-1}i\alpha e^{-2iky}; \qquad k \geq 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}. \tag{3.4.6}$$

The unitary *on-shell scattering matrix* $\mathcal{S}_{\alpha,y}(k)$ in $\mathbb{C}^2$ which is defined by

$$\mathcal{S}_{\alpha,y}(k) = \begin{bmatrix} \mathcal{T}^{\mathrm{l}}_{\alpha,y}(k) & \mathcal{R}^{\mathrm{r}}_{\alpha,y}(k) \\ \mathcal{R}^{\mathrm{l}}_{\alpha,y}(k) & \mathcal{T}^{\mathrm{r}}_{\alpha,y}(k) \end{bmatrix}, \qquad k \geq 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}, \tag{3.4.7}$$

then simply reads

$$\mathcal{S}_{\alpha,y}(k) = (2k+i\alpha)^{-1}\begin{bmatrix} 2k & -i\alpha e^{-2iky} \\ -i\alpha e^{2iky} & 2k \end{bmatrix},$$

$$k \geq 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}. \tag{3.4.8}$$

We note that in the low-energy limit $k \to 0$ (resp. in the high-energy limit $k \to \infty$)

$$\begin{aligned}
&\mathcal{S}_{\alpha,y}(k) \xrightarrow[k\to 0]{} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \qquad y \in \mathbb{R}, \quad -\infty < \alpha \leq \infty, \quad \alpha \neq 0,\\
&\mathcal{S}_{\alpha,y}(k) \xrightarrow[k\to\infty]{} 1, \qquad \alpha, y \in \mathbb{R}.
\end{aligned} \tag{3.4.9}$$

Obviously, $\mathscr{S}_{\alpha,y}(k)$ has a meromorphic continuation to all of $\mathbb{C}$ such that the pole of $\mathscr{S}_{\alpha,y}(k)$ coincides with the bound state ($\alpha < 0$) or resonance ($\alpha > 0$) of $-\Delta_{\alpha,y}$.

For an illustration of $|\mathscr{T}_{\alpha,y}(k)|^2 \equiv |\mathscr{T}^{\mathrm{r}(1)}_{\alpha,y}(k)|^2$, cf. Figure 40(a) [397] in Sect. III.2.3, p. 275.

The above approach is an entirely stationary one, the relation to time-dependent scattering theory is described in Appendix E.

Next, we briefly discuss stationary scattering theory associated with $H_{\varepsilon,y}$. Let u and v be as in Sect. 3.2 and introduce in $L^2(\mathbb{R})$ the states

$$\begin{aligned} &\Phi^-_{\varepsilon,y}(k,\sigma,x) = u_\varepsilon(x)e^{ik\sigma x}, \\ &\Phi^+_{\varepsilon,y}(k,\sigma,x) = v_\varepsilon(x)e^{ik\sigma x}; \qquad \varepsilon > 0, \quad k \geq 0, \end{aligned} \tag{3.4.10}$$

where

$$u_\varepsilon(x) = u((x-y)/\varepsilon), \qquad v_\varepsilon(x) = v((x-y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}. \tag{3.4.11}$$

The *transition operator* $t_\varepsilon(k)$ is then defined as

$$\begin{aligned} &t_\varepsilon(k) = \varepsilon^{-2}\lambda(\varepsilon)[1 + \varepsilon^{-2}\lambda(\varepsilon)u_\varepsilon G_k v_\varepsilon]^{-1}, \\ &\qquad \varepsilon > 0, \quad \operatorname{Im} k \geq 0, \quad k \neq 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \end{aligned} \tag{3.4.12}$$

where $\lambda(\cdot)$ has been introduced in Sect. 3.2,

$$\begin{aligned} &\mathscr{E}_\varepsilon = \{k^2 \in \mathbb{C} - \{0\} \,|\, \lambda(\varepsilon)uG_{\varepsilon k}v\phi_\varepsilon = -\phi_\varepsilon \text{ for some } \phi_\varepsilon \in L^2(\mathbb{R}), \phi_\varepsilon \neq 0, \operatorname{Im} k \geq 0\}, \\ &\qquad \varepsilon > 0, \end{aligned} \tag{3.4.13}$$

and the *on-shell scattering amplitude* $f_{\varepsilon,y,\sigma\sigma'}(k)$ reads

$$\begin{aligned} &f_{\varepsilon,y,\sigma\sigma'}(k) = (2ik)^{-1}(\Phi^+_{\varepsilon,y}(k,\sigma), t_\varepsilon(k)\Phi^-_{\varepsilon,y}(k,\sigma')), \\ &\qquad \varepsilon, k > 0, \quad \sigma, \sigma' = \pm 1, \quad y \in \mathbb{R}. \end{aligned} \tag{3.4.14}$$

(Using Jost function techniques one can show that $\mathscr{E}_\varepsilon \cap (0,\infty) = \varnothing$ (cf., e.g., [122], Ch. XVII).) The unitary *on-shell scattering matrix* $S_{\varepsilon,y}(k) = [S_{\varepsilon,y,\sigma\sigma'}(k)]_{\sigma,\sigma'=\pm 1}$ in $\mathbb{C}^2$ associated with $H_{\varepsilon,y}$ is then simply defined as

$$S_{\varepsilon,y,\sigma\sigma'}(k) = \delta_{\sigma\sigma'} + f_{\varepsilon,y,\sigma\sigma'}(k), \qquad \varepsilon, k > 0, \quad \sigma, \sigma' = \pm 1, \quad y \in \mathbb{R}. \tag{3.4.15}$$

In particular, the *transmission* and *reflection coefficients* ([122], Ch. XVII) corresponding to $H_{\varepsilon,y}$ are given by

$$\begin{aligned} &T^{\mathrm{l}}_{\varepsilon,y}(k) = S_{\varepsilon,y,++}(k) = S_{\varepsilon,y,--}(k) = T^{\mathrm{r}}_{\varepsilon,y}(k), \\ &R^{\mathrm{l}}_{\varepsilon,y}(k) = S_{\varepsilon,y,-+}(k), \qquad R^{\mathrm{r}}_{\varepsilon,y}(k) = S_{\varepsilon,y,+-}(k); \qquad \varepsilon, k > 0, \quad y \in \mathbb{R}. \end{aligned} \tag{3.4.16}$$

After these preliminaries we are able to state our main result concerning the expansion of the on-shell scattering matrix $S_{\varepsilon,y}(k)$ around its limit $\mathscr{S}_{\alpha,y}(k)$ as $\varepsilon \to 0$:

Theorem 3.4.1. *Assume* $V \in L^1(\mathbb{R})$ *to be real-valued and let* $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x)$, $y \in \mathbb{R}$. *Then* $S_{\varepsilon,y}(k)$, $k > 0$, *converges to* $\mathscr{S}_{\alpha,y}(k)$ *as* $\varepsilon \downarrow 0$. *If, in* *addition, $e^{2a|\cdot|}V \in L^1(\mathbb{R})$ for some $a > 0$, then $S_{\varepsilon,y}(k)$ is analytic in ε near $\varepsilon = 0$ and we obtain the expansion*

$$S_{\varepsilon,y}(k) \underset{\varepsilon\to 0}{=} \mathscr{S}_{\alpha,y}(k) + \varepsilon S_y^{(1)}(k) + O(\varepsilon^2), \qquad \alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x), \quad k > 0, \tag{3.4.17}$$

where

$$\begin{aligned} S^{(1)}_{\varepsilon,y,++}(k) = S^{(1)}_{\varepsilon,y,--}(k) = (2k + i\alpha)^{-1}\{&(2k + i\alpha)^{-1} 2ik\lambda'(0)(v, Nu) \\ &-(2k + i\alpha)^{-1}(\alpha/2)\lambda''(0)(v, u) - (i/2)\lambda''(0)(v, u) \\ &+ k\lambda'(0)[(v, ux') - (vx, u)]\}, \end{aligned} \tag{3.4.18}$$

$$\begin{aligned} S^{(1)}_{\varepsilon,y,\mp\pm}(k) = (2k + i\alpha)^{-1} e^{\pm 2iky}\{&(2k + i\alpha)^{-1} 2ik\lambda'(0)(v, Nu) \\ &-(2k + i\alpha)^{-1}(\alpha/2)\lambda''(0)(v, u) - (i/2)\lambda''(0)(v, u) \\ &\pm k\lambda'(0)[(v, ux') + (vx, u)]\}. \end{aligned} \tag{3.4.19}$$

Here the kernel of the Hilbert–Schmidt operator N has been defined in (3.3.10), *and $+$ or $-$ on the right-hand side of* (3.4.19) *corresponds to the reflection coefficient from the left or from the right, respectively.*

PROOF. It suffices to treat the transmission coefficient $T^{r}_{\varepsilon,y}(k) = T^{l}_{\varepsilon,y}(k) \equiv T_{\varepsilon,y}(k)$. By a translation $x \to x + y$ and a scaling transformation $x \to \varepsilon x$, using (3.2.18) we get

$$\begin{aligned} T_{\varepsilon,y}(k) &= 1 + (2ik)^{-1}(\Phi^{+}_{\varepsilon,y}(k, +1), t_{\varepsilon}(k)\Phi^{-}_{\varepsilon,y}(k, +1)) \\ &= 1 + (2i\varepsilon k)^{-1}\lambda(\varepsilon)(ve^{i\varepsilon kx}, [1 + \lambda(\varepsilon)uG_{\varepsilon k}v]^{-1}ue^{i\varepsilon kx'}), \qquad \varepsilon, k > 0, \end{aligned} \tag{3.4.20}$$

where in obvious notation x and x' denote integration variables. Assume that $e^{2a|\cdot|}V \in L^1(\mathbb{R})$ for some $a > 0$. Then

$$\lambda(\varepsilon)uG_{\varepsilon k}v = (i/2k)\lambda'(0)(v, \cdot)u - \varepsilon N + \varepsilon(i/4k)(v, \cdot)u + O(\varepsilon^2), \qquad k > 0, \tag{3.4.21}$$

is analytic in Hilbert–Schmidt norm around $\varepsilon = 0$ (cf. the discussion following (3.3.6)). Applying formula (1.3.47) we immediately infer that $[1 + \lambda(\varepsilon)uG_{\varepsilon k}v]^{-1}$ and hence the right-hand side of (3.4.20) is analytic in ε near $\varepsilon = 0$. The result (3.4.18) then simply follows by a straightforward Taylor expansion of all quantities in (3.4.20) with respect to ε near $\varepsilon = 0$. Similarly, if $V \in L^1(\mathbb{R})$, one proves by dominated convergence that

$$\lim_{\varepsilon\downarrow 0} \|\lambda(\varepsilon)uG_{\varepsilon k}v - (i/2k)\lambda'(0)(v, \cdot)u\|_2 = 0, \qquad k > 0. \tag{3.4.22}$$

Thus

$$\begin{aligned} \operatorname*{n-lim}_{\varepsilon\downarrow 0} [1 + \lambda(\varepsilon)uG_{\varepsilon k}v]^{-1} &= [1 - (i/2k)\lambda'(0)(v, \cdot)u]^{-1} \\ &= 1 - [-i2k(\lambda'(0))^{-1} + (v, u)]^{-1}(v, \cdot)u \end{aligned} \tag{3.4.23}$$

by applying (1.3.47) again. Inserting (3.4.23) into (3.4.20) finally yields

$$\begin{aligned} \lim_{\varepsilon\downarrow 0} T_{\varepsilon,y}(k) &= 1 + (2ik)^{-1}\lambda'(0)(v, \{1 - [-2ik(\lambda'(0))^{-1} + (v, u)]^{-1}(v, \cdot)u\}u) \\ &= \mathscr{T}_{\alpha,y}(k), \qquad k > 0, \end{aligned} \tag{3.4.24}$$

with $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\, V(x)$. ■

We note that, in analogy to our considerations in Sect. 3.2, $S_{\varepsilon,y}(k)$ converges to 1 as $\varepsilon \downarrow 0$ if and only if $\alpha = \lambda'(0) \int_{\mathbb{R}} dx\, V(x) = 0$, i.e., if the δ-interaction at the point y actually disappears.

As in Sects. 3.1 and 3.2 the above results directly extend to the case of complex δ-interactions with $\operatorname{Im} \alpha < 0$. In this case $\mathcal{S}_{\alpha,y}(k)$ and $S_{\varepsilon,y}(k)$ become contractions in $\mathbb{C}^2$.

Notes

Section I.3.1

The one-center point interaction in one dimension has been studied, e.g., in [21], [41], [47], [106], [107], [112], [133], [172], [177], p. 28, [187], [188], [220], [371], [510], [511], [512]. Self-adjoint extensions of symmetric operators, particularly in the context of point interactions, are treated in [184], [512]. The quadratic form approach to defining Hamiltonians is extensively discussed in [283], Ch. VI; [389], Ch. X; [434], Ch. II. The reformulation of Schrödinger dynamics in terms of local Dirichlet forms has been reviewed in [462] (see also [25], [106], [107], [495], [496] and Appendix F). We also mention another possibility of introducing δ-interactions in $L^2(\mathbb{R})$. Let

$$A_y = \frac{d}{dx} + (\alpha/2)\varepsilon_y, \qquad \mathcal{D}(A_y) = H^{2,1}(\mathbb{R}), \qquad \alpha, y \in \mathbb{R},$$

where

$$\varepsilon_y(x) = \begin{cases} 1, & x > y, \\ -1, & x < y. \end{cases}$$

Then

$$A_y^* = -\frac{d}{dx} + (\alpha/2)\varepsilon_y, \qquad \mathcal{D}(A_y^*) = H^{2,1}(\mathbb{R})$$

and by a simple computation

$$A_y A_y^* = -\Delta_{\alpha,y} + (\alpha^2/4), \qquad A_y^* A_y = -\Delta_{-\alpha,y} + (\alpha^2/4).$$

Finally, we note that an appropriate Laplace transform of (3.1.16) explicitly yields the semigroup integral kernel associated with $-\Delta_{\alpha,y}$:

$$\begin{aligned} &e^{-z(-\Delta_{\alpha,y})}(x, x') \\ &\quad = (4\pi z)^{-1/2} e^{-|x-x'|^2/4z} - (\alpha/2) \exp\{(\alpha^2 z/4) + (\alpha[|x-y| + |x'-y|]/2)\} \cdot \\ &\qquad \cdot \{[1 - \Phi(2^{-1} z^{1/2}[\alpha + z^{-1}(|x-y| + |x'-y|)])] + \theta(-\alpha)\}, \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \operatorname{Re} z > 0, \end{aligned}$$

where $\Phi(\cdot)$ denotes the error function [1] and

$$\theta(\mu) = \begin{cases} 1, & \mu > 0, \\ 0, & \mu \le 0. \end{cases}$$

The corresponding unitary group $e^{-it(-\Delta_{\alpha,y})}$ is obtained after the substitution

$$z \to it, \qquad (it)^{1/2} = |t|^{1/2} \begin{cases} e^{i\pi/4}, & t > 0, \\ e^{-i\pi/4}, & t < 0. \end{cases}$$

An integral representation for the above integral kernel has been derived in [195] (cf. also [412]).

A Feynman path integral approach to $-\Delta_{\alpha,y}$ appeared in [218].

The Stark effect in connection with $-\Delta_{\alpha,y}$ is considered in [36].

Section I.3.2

This section closely follows [21], where the first proof of norm resolvent convergence towards point interactions in one dimension has been derived. For earlier results on strong resolvent convergence using local interactions we refer to [187], [188]. Separable interactions are discussed in [112], [129], and [512]. For recent approximation results for more general systems of the type $-d^2/dx^2 + V(x) + \alpha\delta(x)$, cf. [171], [415], [417].

Section I.3.3

Here the whole treatment is taken from Albeverio, Gesztesy, Høegh-Krohn, and Kirsch [21]. Since by eq. (3.2.14) $\varepsilon^2 H_{\varepsilon,y}$ is unitarily equivalent to $H_y(\varepsilon)$, and the latter is unitarily equivalent to $-\Delta \dotplus \lambda(\varepsilon)V(\cdot)$ (just by translations), and $\lambda(\varepsilon) = O(\varepsilon)$ as $\varepsilon \to 0$, the results on bound states of $H_{\varepsilon,y}$ could have been derived directly from the detailed analysis of Klaus [293] and Simon [435] on weakly coupled Schrödinger operators in one dimension. In particular, our main tool for using Fredholm determinants is taken from [435]. If the potential is not exponentially decreasing at infinity, analyticity of k_ε around $\varepsilon = 0$ in (3.3.3) and (3.3.4) is lost. Instead, one obtains asymptotic expansions (the order of which depends on the decrease of V at infinity) as shown in [293], [294], [296].

Section I.3.4

Scattering theory in connection with δ-interactions has been discussed, e.g., in [47a], [156], [173], [200], [218], [314], [315], [347], [379], and [387]. Our brief summary of stationary scattering theory for Schrödinger operators on the line is taken from [100], [142], and [359]. The first part of Theorem 3.4.1 appeared in [379]. We also remark that the assumption $(1 + |x|^m)V \in L^1(\mathbb{R})$ for suitable $m \in \mathbb{N}$ turns the analytic expansion for $S_{\varepsilon,y}(k)$ around $\varepsilon = 0$ into an asymptotic one, the order of which depends on m.

CHAPTER I.4

The One-Center δ'-Interaction in One Dimension

While there is one kind of point interaction in two and three dimensions, we will show in this chapter that there are more possibilities in one dimension.

First, we have the point interaction corresponding to a δ-function, i.e., similar to the two- and three-dimensional cases which we exhibited in Ch. 3. In addition, we will now derive the existence of a four-parameter family of self-adjoint extensions of a symmetric operator with boundary conditions at a particular point in $\mathbb{R}$. However, here we will treat only the one-parameter family corresponding to a δ'-interaction.

We briefly describe basic properties of the δ'-interaction in one dimension. Since the technical tools needed in the proofs are identical to those in Sects. 3.1 and 3.4 we essentially skip the details.

In the Hilbert space $L^2(\mathbb{R})$ we define the closed and nonnegative operator $\ddot{H}_y$ as

$$\ddot{H}_y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\ddot{H}_y) = \{g \in H^{2,2}(\mathbb{R}) | g(y) = g'(y) = 0\} = H_0^{2,2}(\mathbb{R} - \{y\}) \quad \text{for some} \quad y \in \mathbb{R}, \tag{4.1}$$

whose adjoint is given by

$$\ddot{H}_y^* = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\ddot{H}_y^*) = H^{2,2}(\mathbb{R} - \{y\}), \qquad y \in \mathbb{R}. \tag{4.2}$$

A straightforward calculation shows that the equation

$$\ddot{H}_y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\ddot{H}_y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{4.3}$$

has the solutions

$$\psi_1(k, x) = \begin{cases} e^{ik(x-y)}, & x > y, \\ 0, & x < y, \end{cases} \quad \psi_2(k, x) = \begin{cases} 0, & x > y, \\ e^{ik(y-x)}, & x < y, \end{cases} \quad \operatorname{Im} k > 0. \tag{4.4}$$

Thus $\ddot{H}_y$ has deficiency indices (2, 2) and hence it has a four-parameter family of self-adjoint extensions. We are particularly interested in a special one-parameter family of self-adjoint extensions $\Xi_{\beta,y}$ defined by

$$\Xi_{\beta,y} = -\frac{d^2}{dx^2},$$

$$\mathscr{D}(\Xi_{\beta,y}) = \{g \in H^{2,2}(\mathbb{R} - \{y\}) | g'(y+) = g'(y-), g(y+) - g(y-) = \beta g'(y)\},$$
$$-\infty < \beta \leq \infty. \tag{4.5}$$

The special case $\beta = 0$ leads to the kinetic energy Hamiltonian $-\Delta$ in $L^2(\mathbb{R})$. The case $\beta = \infty$ leads to a Neumann boundary condition at y and decouples $(-\infty, y)$ and (y, ∞), viz.

$$\mathscr{D}(\Xi_{\infty,y}) = \{g \in H^{2,2}(\mathbb{R} - \{y\}) | g'(y+) = g'(y-) = 0\}$$
$$= \mathscr{D}(-\Delta_{N-}) \oplus \mathscr{D}(-\Delta_{N+}), \tag{4.6}$$

$$\Xi_{\infty,y} = (-\Delta_{N-}) \oplus (-\Delta_{N+}), \tag{4.7}$$

where $-\Delta_{N\pm}$ denotes the Neumann Laplacian on $(y, \pm\infty)$,

$$\mathscr{D}(-\Delta_{N\pm}) = \{g \in H^{2,2}((y, \pm\infty)) | g'(y\pm) = 0\}. \tag{4.8}$$

By definition, $\Xi_{\beta,y}$ describes a δ'-interaction centered at $y \in \mathbb{R}$. The resolvent of $\Xi_{\beta,y}$ is described in

Theorem 4.1. *The resolvent of $\Xi_{\beta,y}$ is given by*

$$(\Xi_{\beta,y} - k^2)^{-1} = G_k - 2\beta k^2(2 - i\beta k)^{-1}(\overline{\tilde{\tilde{G}}_k(\cdot - y)}, \cdot)\tilde{\tilde{G}}_k(\cdot - y),$$
$$k^2 \in \rho(\Xi_{\beta,y}), \quad \operatorname{Im} k > 0, \quad -\infty < \beta \leq \infty, \quad y \in \mathbb{R}, \tag{4.9}$$

with integral kernel

$$(\Xi_{\beta,y} - k^2)^{-1}(x, x')$$
$$= (i/2k)e^{ik|x-x'|}$$
$$+ (\beta/2)(2 - i\beta k)^{-1}\begin{Bmatrix} e^{ik(x-y)}, & x > y \\ -e^{ik(y-x)}, & x < y \end{Bmatrix} \cdot \begin{Bmatrix} e^{ik(x'-y)}, & x' > y \\ -e^{ik(y-x')}, & x' < y \end{Bmatrix},$$
$$k^2 \in \rho(\Xi_{\beta,y}), \quad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}, \tag{4.10}$$

where

$$\tilde{\tilde{G}}_k(x - y) = (i/2k)\begin{cases} e^{ik(x-y)}, & x > y, \\ -e^{ik(y-x)}, & x < y, \end{cases} \quad \operatorname{Im} k > 0. \tag{4.11}$$

PROOF. Krein's formula (cf. Theorem A.3) implies

$$(\Xi_{\beta,y} - k^2)^{-1} = G_k - (4k^2)^{-1} \sum_{l,m=1}^{2} \lambda_{lm}(k)(\psi_m(-\bar{k}), \cdot)\psi_l(k). \tag{4.12}$$

By taking the adjoint of (4.12) one infers

$$\lambda_{lm}(-\bar{k}) = \overline{\lambda_{ml}(k)}. \tag{4.13}$$

Next, let $g \in L^2(\mathbb{R})$ and define

$$h_\beta(x) = ((-\Delta - k^2)^{-1}g)(x) - \lambda_{11}(k)(4k^2)^{-1}e^{ik(x-y)} \int_y^\infty dx'\, e^{ik(x'-y)}g(x')$$
$$-\lambda_{12}(k)(4k^2)^{-1}e^{ik(x-y)} \int_{-\infty}^y dx'\, e^{ik(y-x')}g(x'), \qquad x > y,$$
$$h_\beta(x) = ((-\Delta - k^2)^{-1}g)(x) - \lambda_{22}(k)(4k^2)^{-1}e^{ik(y-x)} \int_{-\infty}^y dx'\, e^{ik(y-x')}g(x')$$
$$-\lambda_{21}(k)(4k^2)^{-1}e^{ik(y-x)} \int_y^\infty dx'\, e^{ik(x'-y)}g(x'), \qquad x < y. \tag{4.14}$$

After imposing the boundary conditions

$$h'_\beta(y+) = h'_\beta(y-), \qquad h_\beta(y+) - h_\beta(y-) = \beta h'_\beta(y) \tag{4.15}$$

one obtains

$$\lambda(k) = -2\beta k^2(2 - i\beta k)^{-1}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \tag{4.16}$$

Note that $\det[\lambda(k)] \equiv 0$ (cf. the discussion in the Notes). In fact, by inserting (4.16) into (4.12) the expression (4.12) reduces to (4.9). ■

Further information about $\Xi_{\beta,y}$ is contained in

Theorem 4.2. *The domain $\mathscr{D}(\Xi_{\beta,y})$, $-\infty < \beta \le \infty$, $y \in \mathbb{R}$, consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) - 2i\beta k(2 - i\beta k)^{-1}\phi'_k(y)\tilde{\tilde{G}}_k(x - y), \tag{4.17}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ and $k^2 \in \rho(\Xi_{\beta,y})$, $\operatorname{Im} k > 0$. The decomposition (4.17) is unique and with $\psi \in \mathscr{D}(\Xi_{\beta,y})$ of this form we obtain

$$(\Xi_{\beta,y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{4.18}$$

Next, let $\psi \in \mathscr{D}(\Xi_{\beta,y})$ and suppose that $\psi = 0$ in an open set $U \subseteq \mathbb{R}$. Then $\Xi_{\beta,y}\psi = 0$ in U, i.e., $\Xi_{\beta,y}$ describes a local interaction.

PROOF. Identical to that of Theorem 3.1.3. ■

Spectral properties of $\Xi_{\beta,y}$ are summarized in

Theorem 4.3. *Let* $-\infty < \beta \le \infty$, $y \in \mathbb{R}$. *Then the essential spectrum of* $\Xi_{\beta,y}$ *is purely absolutely continuous and covers the nonnegative real axis*

$$\sigma_{\text{ess}}(\Xi_{\beta,y}) = \sigma_{\text{ac}}(\Xi_{\beta,y}) = [0, \infty), \qquad \sigma_{\text{sc}}(\Xi_{\beta,y}) = \varnothing. \tag{4.19}$$

If $-\infty < \beta < 0$, $\Xi_{\beta,y}$ *has precisely one negative, simple eigenvalue, i.e., its point spectrum* $\sigma_{\text{p}}(\Xi_{\beta,y})$ *reads*

$$\sigma_{\text{p}}(\Xi_{\beta,y}) = \{-4/\beta^2\}, \qquad -\infty < \beta < 0, \tag{4.20}$$

with

$$(-\beta/8)^{1/2}\begin{cases} e^{(2/\beta)(x-y)}, & x > y, \\ -e^{(2/\beta)(y-x)}, & x < y, \end{cases} \qquad -\infty < \beta < 0, \tag{4.21}$$

its (normalized) eigenfunction. For $\beta \ge 0$ *or* $\beta = \infty$, $\Xi_{\beta,y}$ *has no eigenvalues*

$$\sigma_p(\Xi_{\beta,y}) = \varnothing, \qquad \beta \notin (-\infty, 0). \tag{4.22}$$

PROOF. Analogous to that of Theorem 3.1.4. ∎

Again the pole structure of (4.10) determines bound states and resonances of $\Xi_{\beta,y}$: For $\beta > 0$, $\Xi_{\beta,y}$ has a simple resonance at $k_0 = -2i/\beta$ with resonance function

$$\psi_{k_0}(x) = \begin{cases} e^{(2/\beta)(x-y)}, & x > y, \\ -e^{(2/\beta)(y-x)}, & x < y, \end{cases} \qquad \beta > 0.$$

For all $-\infty < \beta < \infty$, $\Xi_{\beta,y}$ has, in addition, a simple zero-energy resonance (in contrast to $-\Delta_{\alpha,y}$, the first-order pole in (4.10) at $k = 0$ does not cancel) with resonance function $\psi_0(x) = 1$. For $\beta = \infty$, $\Xi_{\beta,y}$ has a zero-energy resonance of multiplicity two with corresponding resonance functions

$$\psi_{01}(x) = \begin{cases} 1, & x > y, \\ 0, & x < y. \end{cases} \qquad \psi_{02}(x) = \begin{cases} 0, & x > y, \\ 1, & x < y. \end{cases}$$

It remains to discuss stationary scattering theory associated with the pair $(\Xi_{\beta,y}, -\Delta)$. The generalized eigenfunctions of $\Xi_{\beta,y}$ are given by

$$\Psi_{\beta,y}(k,\sigma,x) = e^{ik\sigma x} + i\beta k\sigma(2 - i\beta k)^{-1} e^{ik\sigma y}\begin{cases} e^{ik(x-y)}, & x > y, \\ -e^{ik(y-x)}, & x < y, \end{cases}$$

$$k \ge 0, \quad \sigma = \pm 1, \quad -\infty < \beta \le \infty, \quad x, y \in \mathbb{R}. \tag{4.23}$$

They fulfill

$$\begin{aligned} &\Psi'_{\beta,y}(k, \sigma, y+) = \Psi'_{\beta,y}(k, \sigma, y-), \\ &\Psi_{\beta,y}(k, \sigma, y+) - \Psi_{\beta,y}(k, \sigma, y-) = \beta\Psi'_{\beta,y}(k, \sigma, y), \\ &-\Psi''_{\beta,y}(k, \sigma, x) = k^2\Psi_{\beta,y}(k, \sigma, x), \qquad x \in \mathbb{R} - \{y\}, \\ &\lim_{\varepsilon \downarrow 0}\lim_{x' \to -\infty} (2k/i)e^{\pm i(k+i\varepsilon)x'}[\Xi_{\beta,y} - (k + i\varepsilon)^2]^{-1}(x, x') = \Psi_{\beta,y}(k, \pm 1, x), \\ &\qquad x \in R; \quad k \ge 0. \end{aligned} \tag{4.24}$$

The corresponding *transmission* and *reflection coefficients* from the left and right then read

$$\mathscr{T}^{1}_{\beta,y}(k) = \lim_{x\to+\infty} e^{-ikx}\Psi_{\beta,y}(k, +1, x) = 2(2 - i\beta k)^{-1}, \tag{4.25}$$

$$\mathscr{T}^{\mathrm{r}}_{\beta,y}(k) = \lim_{x\to-\infty} e^{ikx}\Psi_{\beta,y}(k, -1, x) = 2(2 - i\beta k)^{-1}, \tag{4.26}$$

$$\mathscr{R}^{1}_{\beta,y}(k) = \lim_{x\to-\infty} e^{ikx}[\Psi_{\beta,y}(k, +1, x) - e^{ikx}] = -(2 - i\beta k)^{-1} i\beta k e^{2iky}, \tag{4.27}$$

$$\mathscr{R}^{\mathrm{r}}_{\beta,y}(k) = \lim_{x\to+\infty} e^{-ikx}[\Psi_{\beta,y}(k, -1, x) - e^{-ikx}] = -(2 - i\beta k)^{-1} i\beta k e^{-2iky};$$

$$k \geq 0, \quad -\infty < \beta \leq \infty, \quad y \in \mathbb{R}. \tag{4.28}$$

The unitary *on-shell scattering matrix* $\mathscr{S}_{\beta,y}(k)$ in $\mathbb{C}^2$ is then given by

$$\begin{aligned}\mathscr{S}_{\beta,y}(k) &= \begin{bmatrix} \mathscr{T}^{1}_{\beta,y}(k) & \mathscr{R}^{\mathrm{r}}_{\beta,y}(k) \\ \mathscr{R}^{1}_{\beta,y}(k) & \mathscr{T}^{\mathrm{r}}_{\beta,y}(k) \end{bmatrix} \\ &= (2 - i\beta k)^{-1} \begin{bmatrix} 2 & -i\beta k e^{-2iky} \\ -i\beta k e^{2iky} & 2 \end{bmatrix},\end{aligned}$$

$$k \geq 0, \quad -\infty < \beta \leq \infty, \quad y \in \mathbb{R}. \tag{4.29}$$

In the low-energy limit $k \to 0$ we get

$$\begin{aligned}&\mathscr{S}_{\beta,y}(k) \underset{k\to 0}{\longrightarrow} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad -\infty < \beta < \infty, \\ &\mathscr{S}_{\infty,y}(k) \underset{k\to 0}{\longrightarrow} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.\end{aligned} \tag{4.30}$$

Obviously, $\mathscr{S}_{\beta,y}(k)$ has a meromorphic continuation in k to all of $\mathbb{C}$ such that for $k \neq 0$ the pole of $\mathscr{S}_{\beta,y}(k)$ coincides with the bound state ($\beta < 0$) or resonance ($\beta > 0$) of $\Xi_{\beta,y}$.

Notes

The existence of δ'-interactions and their local nature has been pointed out by Grossmann, Høegh-Krohn, and Mebkhout [226]. The first extensive treatment including infinitely many centers appeared in Gesztesy and Holden [205]. The fact that $\det[\lambda(k)] \equiv 0$ in the proof of Theorem 4.1 indicates that $\dot{H}_y$ is not the maximal common part of $\Xi_{\beta,y}$ and $-\Delta$ (cf. Theorem A.3). Indeed, their maximal common part $\dot{H}'_y$ is a proper extension of $\dot{H}_y$ with deficiency indices (1, 1) given by

$$\dot{H}'_y = -\frac{d^2}{dx^2} \quad \text{on} \quad \mathscr{D}(\dot{H}'_y) = \{g \in H^{2,2}(\mathbb{R}) | g'(y) = 0\}.$$

The deficiency subspace of $\dot{H}_y'$ corresponding to $k^2 \in \mathbb{C} - \mathbb{R}$ is spanned by

$$\begin{cases} e^{ik(x-y)}, & x > y, \\ -e^{ik(y-x)}, & x < y, \end{cases} \qquad \operatorname{Im} k > 0,$$

and thus $\Xi_{\beta,y}$, $-\infty < \beta \leq \infty$, are all self-adjoint extensions of $\dot{H}_y'$. Self-adjoint extensions of $\ddot{H}_y$ are considered in [418].

Complex δ'-interaction can be treated in the same way.

Approximations of $\Xi_{\beta,y}$ in the strong resolvent sense by means of scaled rank-one interactions appeared in [419].

More general boundary conditions corresponding to powers of the δ-interaction are studied in [398], [399].

CHAPTER I.5

The One-Center Point Interaction in Two Dimensions

Following Sects. 1.1, 1.4, 2.1, and 2.3 we briefly discuss the point interaction in two dimensions.

Let $y \in \mathbb{R}^2$ and consider in $L^2(\mathbb{R}^2)$ the nonnegative operator

$$-\Delta|_{C_0^\infty(\mathbb{R}^2-\{y\})} \tag{5.1}$$

with $\dot{H}_y$ its closure in $L^2(\mathbb{R}^2)$ (i.e., $\mathscr{D}(\dot{H}_y) = H_0^{2,2}(\mathbb{R}^2 - \{y\})$). Then its adjoint $\dot{H}_y^*$ reads

$$\dot{H}_y^* = -\Delta, \qquad \mathscr{D}(\dot{H}^*) = \{g \in H_{\text{loc}}^{2,2}(\mathbb{R}^2 - \{y\}) \cap L^2(\mathbb{R}^2) | \Delta g \in L^2(\mathbb{R}^2)\},$$
$$y \in \mathbb{R}^2. \tag{5.2}$$

A direct calculation shows that the equation

$$\dot{H}_y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{5.3}$$

has the unique solution

$$\psi(k, x) = (i/4) H_0^{(1)}(k|x - y|), \qquad x \in \mathbb{R}^2 - \{y\}, \quad \operatorname{Im} k > 0, \tag{5.4}$$

where $H_0^{(1)}(\cdot)$ denotes the Hankel function of first kind and order zero [1]. As a consequence $\dot{H}_y$ has deficiency indices (1, 1). In order to determine all self-adjoint extensions of $\dot{H}_y$ we decompose $L^2(\mathbb{R}^2)$ with respect to angular momenta

$$L^2(\mathbb{R}^2) = L^2((0, \infty); r\, dr) \otimes L^2(S^1), \tag{5.5}$$

where S^1 denotes the unit sphere in $\mathbb{R}^2$. Using the unitary transformation

$$\tilde{U}: L^2((0, \infty); r\, dr) \to L^2([0, \infty); dr), \qquad (\tilde{U}f)(r) = r^{1/2} f(r) \tag{5.6}$$

and the fact that $\{Y_m(\omega) = (2\pi)^{-1/2} e^{im\theta} | m \in \mathbb{Z}, 0 < \theta < 2\pi, \omega = (\cos\theta, \sin\theta)\}$ provides a basis for $L^2(S^1)$, we can rewrite (5.5) as

$$L^2(\mathbb{R}^2) = \bigoplus_{m=-\infty}^{\infty} \tilde{U}^{-1} L^2((0, \infty); dr) \otimes [Y_m]. \tag{5.7}$$

With respect to this decomposition $\dot{H}_y$ equals the direct sum

$$\dot{H}_y = T_y^{-1} \left\{ \bigoplus_{m=-\infty}^{\infty} \tilde{U}^{-1} \dot{h}_m \tilde{U} \otimes 1 \right\} T_y, \qquad y \in \mathbb{R}^2, \tag{5.8}$$

where $(T_y g)(x) = g(x + y)$, $g \in L^2(\mathbb{R}^2)$, and

$$\dot{h}_m = -\frac{d^2}{dr^2} + \frac{m^2 - 4^{-1}}{r^2}, \qquad r > 0, \quad m \in \mathbb{Z},$$

$$\begin{aligned} \mathscr{D}(\dot{h}_0) = \{&\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\text{loc}}((0, \infty)); W(\phi, \phi_\pm)_{0+} = 0; \\ &- \phi'' - 4^{-1} r^{-2} \phi \in L^2((0, \infty))\}, \\ \mathscr{D}(\dot{h}_m) = \{&\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\text{loc}}((0, \infty)); \\ &-\phi'' + (m^2 - \tfrac{1}{4}) r^{-2} \phi \in L^2((0, \infty))\}, \qquad m \in \mathbb{Z} - \{0\}. \end{aligned} \tag{5.9}$$

Here $AC_{\text{loc}}((a, b))$ denotes the set of locally absolutely continuous functions on (a, b), $W(f, g)_x = \overline{f(x)} g'(x) - \overline{f'(x)} g(x)$ denotes the Wronskian of f and g, and $\phi_\pm(r) = r^{1/2} H_0^{(1)}((\pm i)^{1/2} r)$. As is well known (e.g., [389], Ch. X) $\dot{h}_m$, $m \in \mathbb{Z} - \{0\}$, are self-adjoint whereas $\dot{h}_0$ has deficiency indices (1, 1). All self-adjoint extensions of $\dot{h}_0$ may be parametrized by (cf. Appendix D)

$$h_{0,\alpha} = -\frac{d^2}{dr^2} - \frac{1}{4r^2}, \qquad r > 0,$$

$$\begin{aligned} \mathscr{D}(h_{0,\alpha}) = \{&\phi \in L^2((0, \infty)) | \phi, \phi' \in AC_{\text{loc}}((0, \infty)); 2\pi\alpha\phi_0 + \phi_1 = 0; \\ &-\phi'' - 4^{-1} r^{-2} \phi \in L^2((0, \infty))\}, \qquad -\infty < \alpha \leq \infty, \end{aligned} \tag{5.10}$$

where ϕ_0 and ϕ_1 are defined as

$$\phi_0 = \lim_{r \downarrow 0} [r^{1/2} \ln r]^{-1} \phi(r), \qquad \phi_1 = \lim_{r \downarrow 0} r^{-1/2} [\phi(r) - \phi_0 r^{1/2} \ln r],$$
$$\phi \in \mathscr{D}(\dot{h}_0^*). \tag{5.11}$$

Thus we get

Theorem 5.1. *All self-adjoint extensions of $\dot{H}_y$ are given by*

$$-\Delta_{\alpha,y} = T_y^{-1} \left\{ \left[\tilde{U}^{-1} h_{0,\alpha} \tilde{U} \oplus \bigoplus_{\substack{m=-\infty \\ m \neq 0}}^{\infty} \tilde{U}^{-1} \dot{h}_m \tilde{U} \right] \otimes 1 \right\} T_y,$$
$$-\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^2. \tag{5.12}$$

The special case $\alpha = \infty$ leads to the kinetic energy Hamiltonian $-\Delta$ (the Friedrichs extension of $\dot{H}_y$) in $L^2(\mathbb{R}^2)$, viz.

$$-\Delta_{\infty,y} = -\Delta, \qquad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2). \tag{5.13}$$

If $|\alpha| < \infty$, $-\Delta_{\alpha,y}$ describes a point interaction centered at $y \in \mathbb{R}^2$. It will turn out later that $(-2\pi\alpha)^{-1}$ represents the scattering length of $-\Delta_{\alpha,y}$.

Next, we note that the integral kernel $G_k(x - x')$ of the free resolvent in $L^2(\mathbb{R}^2)$, i.e.,

$$G_k = (-\Delta - k^2)^{-1}, \qquad \operatorname{Im} k > 0, \tag{5.14}$$

reads

$$G_k(x - x') = (i/4)H_0^{(1)}(k|x - x'|), \quad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}^2, \quad x \neq x'. \tag{5.15}$$

We have

Theorem 5.2. *The resolvent of* $-\Delta_{\alpha,y}$ *is given by*

$$\begin{aligned}(-\Delta_{\alpha,y} - k^2)^{-1} &\\ &= G_k + 2\pi[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}(\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y),\\ &k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, \quad -\infty < \alpha \leq \infty, \quad y \in \mathbb{R}^2, \end{aligned}\tag{5.16}$$

with integral kernel

$$\begin{aligned}(-\Delta_{\alpha,y} - k^2)^{-1}(x, x') &= (i/4)H_0^{(1)}(k|x - x'|)\\ &-(\pi/8)[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}H_0^{(1)}(k|x - y|)H_0^{(1)}(k|y - x'|),\\ k^2 \in \rho(-\Delta_{\alpha,y}), \quad \operatorname{Im} k > 0, &\quad x, x' \in \mathbb{R}^2, \quad x \neq x', \quad x \neq y, \quad x' \neq y. \end{aligned}\tag{5.17}$$

PROOF. By the decomposition (5.12) it suffices to consider the s-wave ($m = 0$). Let $\eta \in L^2((0, \infty))$ and define

$$\begin{aligned}\chi_\alpha(r) &= \int_0^\infty dr'\, g_0(k, r, r')\eta(r')\\ &- (\pi^2/4)[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}\int_0^\infty dr'\,(r')^{1/2}H_0^{(1)}(kr')\eta(r')r^{1/2}H_0^{(1)}(kr),\\ &\operatorname{Im} k > 0, \quad -\infty < \alpha \leq \infty, \end{aligned}\tag{5.18}$$

where

$$g_0(k, r, r') = (i\pi/2)(rr')^{1/2}\begin{cases} J_0(kr)H_0^{(1)}(kr'), & r \leq r',\\ J_0(kr')H_0^{(1)}(kr), & r \geq r',\end{cases} \tag{5.19}$$

is the Green's function corresponding to $h_{0,\infty}$ (the Friedrichs extension of $\dot{h}_0$). Clearly, $\chi_\alpha, \chi_\alpha' \in AC_{\mathrm{loc}}((0, \infty))$ and $\chi_\alpha \in L^2((0, \infty))$. A somewhat lengthy but straightforward calculation then shows that

$$2\pi\alpha(\chi_\alpha)_0 + (\chi_\alpha)_1 = 0, \tag{5.20}$$

and

$$\chi_\alpha''(r) + (4r^2)^{-1}\chi_\alpha(r) = -\eta(r) - k^2\chi_\alpha(r), \qquad r > 0, \tag{5.21}$$

which proves (5.16). ■

Further information on $\mathscr{D}(-\Delta_{\alpha,y})$ and the fact that the one-center point interaction is local is contained in

Theorem 5.3. *The domain $\mathscr{D}(-\Delta_{\alpha,y})$, $-\infty < \alpha \le \infty$, $y \in \mathbb{R}^2$, consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + 2\pi[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}\phi_k(y)G_k(x-y), \qquad x \neq y, \tag{5.22}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2)$ and $k^2 \in \rho(-\Delta_{\alpha,y})$, $\operatorname{Im} k > 0$. The decomposition (5.22) is unique and with $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ of this form we obtain

$$(-\Delta_{\alpha,y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{5.23}$$

Next, let $\psi \in \mathscr{D}(-\Delta_{\alpha,y})$ and assume that $\psi = 0$ in an open set $U \subseteq \mathbb{R}^2$. Then $-\Delta_{\alpha,y}\psi = 0$ in U.

Proof. Identical to that of Theorem 1.1.3. ∎

Concerning spectral properties we have

Theorem 5.4. *Let $-\infty < \alpha \le \infty$, $y \in \mathbb{R}^2$. Then the essential spectrum of $-\Delta_{\alpha,y}$ is purely absolutely continuous and covers the nonegative real axis*

$$\sigma_{\text{ess}}(-\Delta_{\alpha,y}) = \sigma_{\text{ac}}(-\Delta_{\alpha,y}) = [0, \infty), \qquad \sigma_{\text{sc}}(-\Delta_{\alpha,y}) = \varnothing. \tag{5.24}$$

For all $\alpha \in \mathbb{R}$, $-\Delta_{\alpha,y}$ has precisely one negative, simple eigenvalue, i.e., its point spectrum is given by

$$\sigma_{\text{p}}(-\Delta_{\alpha,y}) = \{-4e^{2[-2\pi\alpha + \Psi(1)]}\}, \qquad \alpha \in \mathbb{R}, \tag{5.25}$$

with

$$G_{2i\exp[-2\pi\alpha+\Psi(1)]}(x-y) = (i/4)H_0^{(1)}[2ie^{[-2\pi\alpha+\Psi(1)]}|x-y|], \quad x \neq y, \tag{5.26}$$

is strictly positive (unnormalized) eigenfunction.

Proof. Similar to that of Theorem 1.1.4. ∎

The pole structure of (5.17) determines bound states and resonances of $-\Delta_{\alpha,y}$: In fact, $(-\Delta_{\alpha,y} - k^2)^{-1}(x, x')$, $x \neq x'$, has a meromorphic continuation to the entire logarithmic Riemann surface. In the cut plane $\{k \in \mathbb{C} - \{0\} \mid -\pi < \arg k < \pi\}$, $-\Delta_{\alpha,y}$ has only the above-mentioned bound state at $k_0 = 2ie^{[-2\pi\alpha+\Psi(1)]}$ but no resonance.

Finally, we turn to stationary scattering theory for the pair $(-\Delta_{\alpha,y}, -\Delta)$. Since $-\Delta_{\alpha,y}$ is invariant under rotations in $\mathbb{R}^2$ with center y we start with the partial wave decomposition (5.12). Let

$$\psi_{0,\alpha}(k, r) = r^{1/2}J_0(kr) + \frac{i\pi}{2}[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}r^{1/2}H_0^{(1)}(kr),$$

$$k > 0, \quad -\infty < \alpha \le \infty, \quad r \ge 0, \tag{5.27}$$

then

$$2\pi\alpha(\psi_{0,\alpha}(k))_0 + (\psi_{0,\alpha}(k))_1 = 0,$$

$$-\psi''_{0,\alpha}(k, r) - (4r^2)^{-1}\psi_{0,\alpha}(k, r) = k^2\psi_{0,\alpha}(k, r), \qquad r > 0,$$

$$\lim_{\varepsilon\downarrow 0}\lim_{r'\to\infty} [2(k + i\varepsilon)/\pi]^{1/2} e^{-i(k+i\varepsilon)r'} e^{-i\pi/4} [h_{0,\alpha} - (k + i\varepsilon)^2]^{-1}(r, r')$$

$$= \psi_{0,\alpha}(k, r), \qquad r \geq 0; \quad k > 0, \quad -\infty < \alpha \leq \infty. \quad (5.28)$$

Thus $\psi_{0,\alpha}(k)$ are generalized eigenfunctions of $h_{0,\alpha}$. For $m \neq 0$ the generalized eigenfunctions of $\dot{h}_m$ read

$$\psi_m(k, r) = r^{1/2} J_m(kr), \qquad k, r \geq 0, \quad m \in \mathbb{Z} - \{0\} \qquad (5.29)$$

(we recall that $J_{-m}(z) = (-1)^m J_m(z)$). The asymptotic behavior of $\psi_{0,\alpha}(k, r)$ as $r \to \infty$ is then given by

$$\psi_{0,\alpha}(k, r) \underset{r\to\infty}{\sim} (2/\pi k)^{1/2} e^{i\delta_{0,\alpha}(k)} \sin[kr + (\pi/4) + \delta_{0,\alpha}(k)],$$

$$k > 0, \quad -\infty < \alpha \leq \infty, \quad (5.30)$$

and

$$\mathcal{S}_{0,\alpha}(k) = e^{2i\delta_{0,\alpha}(k)}$$

$$= [2\pi\alpha - \Psi(1) + \ln(k/2) - (i\pi/2)]^{-1}[2\pi\alpha - \Psi(1) + \ln(k/2) + (i\pi/2)],$$

$$k > 0, \quad -\infty < \alpha \leq \infty, \quad (5.31)$$

denotes the (on-shell) *s-wave scattering matrix* (and $\delta_{0,\alpha}(k)$ the *s-wave scattering phase shift*). For $m \neq 0$, we obtain

$$\mathcal{S}_m(k) = 1, \qquad \delta_m(k) = 0, \qquad m \in \mathbb{Z} - \{0\}. \qquad (5.32)$$

Again it is useful to compare with the *effective range expansion* for spherically symmetric real-valued potentials V satisfying

$$\int_0^\infty dr\, r[1 + |\ln r|]^2 e^{2ar}|V(r)| < \infty \qquad \text{for some } a > 0. \qquad (5.33)$$

If $\delta_m(g, k)$ denote the phase shifts associated with the Schrödinger operators $-d^2/dr^2 + (m^2 - \frac{1}{4})r^{-2} \dotplus gV(r)$ this low-energy expansion reads (cf., e.g., [95], [96])

$$\Gamma(1 + |m|)^{-2}(k/2)^{2|m|}[(\pi/2)\cot\delta_m(g, k) - \ln(k/2) + \Psi(1)]$$

$$= -(a_m(g))^{-1} + r_m(g)k^2 + O(k^4), \qquad k > 0, \quad g \in \mathbb{R}, \quad m \in \mathbb{Z}, \quad (5.34)$$

where the right-hand side of (5.34) is real analytic in k^2 near $k^2 = 0$. The coefficients $a_m(g)$ and $r_m(g)$ are called *partial wave scattering lengths* and *effective range parameters*, respectively.

The explicit relations

$$\begin{aligned} &[(\pi/2)\cot\delta_{0,\alpha}(k) - \ln(k/2) + \Psi(1)] = 2\pi\alpha, \\ &\delta_m(k) = 0, \qquad m \in \mathbb{Z} - \{0\}, \end{aligned} \qquad (5.35)$$

for the point interaction then show that

$$a_{0,\alpha} = (-2\pi\alpha)^{-1}, \qquad -\infty < \alpha \le \infty, \quad \alpha \neq 0, \qquad r_{0,\alpha} \equiv 0, \tag{5.36}$$

and all low-energy parameters vanish identically in higher partial waves $m \in \mathbb{Z} - \{0\}$. We emphasize again that by (5.35) the effective range expansion for $m = 0$ is already exact to zeroth order with respect to k^2. This illustrates the fact that $-\Delta_{\alpha,y}$ describes an s-wave interaction of zero range.

Now we turn to the scattering wave function of $-\Delta_{\alpha,y}$

$$\Psi_{\alpha,y}(k\omega, x) = e^{ik\omega x} + (i\pi/2)[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1} e^{ik\omega y} H_0^{(1)}(k|x-y|),$$
$$k > 0, \quad \omega \in S^1, \quad -\infty < \alpha \le \infty, \quad x, y \in \mathbb{R}^2, \quad x \neq y. \tag{5.37}$$

A comparison of (5.37) with (5.27) and (5.29) yields

$$e^{-ik\omega y}\Psi_{\alpha,y}(k\omega, x) = 2\pi|x-y|^{-1/2}\psi_{0,\alpha}(k|x-y|)\overline{Y_0(\omega)}\,Y_0(\omega_x)$$
$$+ 2\pi|x-y|^{-1/2} \sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty} i^m \psi_m(k|x-y|)\overline{Y_m(\omega)}\,Y_m(\omega_x),$$
$$k > 0, \quad -\infty < \alpha \le \infty, \quad x \neq y, \quad \omega_x = x/|x|, \tag{5.38}$$

by using

$$e^{ik\omega x} = 2\pi \sum_{m=-\infty}^{\infty} i^m J_m(k|x|)\overline{Y_m(\omega)}\,Y_m(\omega_x), \qquad k \ge 0. \tag{5.39}$$

The *on-shell scattering amplitude* $f_{\alpha,y}(k, \omega, \omega')$ corresponding to $-\Delta_{\alpha,y}$ is then given by

$$f_{\alpha,y}(k, \omega, \omega') = \lim_{\substack{|x|\to\infty \\ |x|^{-1}x=\omega}} |x|^{1/2} e^{-ik|x|}[\Psi_{\alpha,y}(k\omega', x) - e^{ik\omega' x}]$$
$$= e^{i\pi/4}(\pi/2k)^{1/2}[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1} e^{ik(\omega'-\omega)y},$$
$$k > 0, \quad \omega, \omega' \in S^1, \quad -\infty < \alpha \le \infty, \quad y \in \mathbb{R}^2. \tag{5.40}$$

The unitary *on-shell scattering operator* $\mathscr{S}_{\alpha,y}(k)$ in $L^2(S^1)$ finally reads

$$\mathscr{S}_{\alpha,y}(k) = 1 + i\pi[2\pi\alpha - \Psi(1) + \ln(k/2i)]^{-1}(e^{-ik(\cdot)y}Y_0, \cdot)e^{-ik(\cdot)y}Y_0,$$
$$k > 0, \quad -\infty < \alpha \le \infty, \quad y \in \mathbb{R}^2. \tag{5.41}$$

The explicit representation (5.41) shows that $\mathscr{S}_{\alpha,y}(k)$ has a meromorphic continuation in k to the entire logarithmic Riemann surface such that its pole in the cut plane $\{k \in \mathbb{C} - \{0\} \mid -\pi < \arg k < \pi\}$ coincides with the bound state of $-\Delta_{\alpha,y}$.

Finally, we emphasize that the ε-expansion for the resolvent, eigenvalues, resonances, scattering amplitude, and the on-shell scattering operator derived in the three-dimensional case works as well in two dimensions. To illustrate these facts its suffices to consider the resolvent.

Let $V\colon \mathbb{R}^2 \to \mathbb{R}$ be measurable and

$$\int_{\mathbb{R}^2} d^2x(1 + |x|^{2+\delta})|V(x)| < \infty, \qquad \int_{\mathbb{R}^2} d^2x|V(x)|^{1+\delta} < \infty$$
$$\text{for some} \quad \delta > 0. \tag{5.42}$$

Again we introduce

$$v(x) = |V(x)|^{1/2}, \qquad u(x) = |V(x)|^{1/2} \operatorname{sgn}[V(x)] \tag{5.43}$$

and note that

$$uG_k v \in \mathscr{B}_2(L^2(\mathbb{R}^2)), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0. \tag{5.44}$$

Let λ: $(0, \varepsilon_0) \to \mathbb{R}$, $\varepsilon_0 > 0$ and

$$\lambda(\mu) = \lambda_1 \mu + \lambda_2 \mu^2 + o(\mu^2). \tag{5.45}$$

Then the form sum

$$H_y(\varepsilon) = -\Delta \dotplus \lambda((\ln \varepsilon)^{-1}) V(\cdot - \varepsilon^{-1} y), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^2, \tag{5.46}$$

in $L^2(\mathbb{R}^2)$ is well defined (cf. Appendix B) and we define the scaled short-range Hamiltonian $H_{\varepsilon,y}$ as

$$\begin{aligned} H_{\varepsilon,y} &= \varepsilon^{-2} U_\varepsilon H_y(\varepsilon) U_\varepsilon^{-1} = -\Delta \dotplus V_{\varepsilon,y}, \\ V_{\varepsilon,y}(x) &= \lambda((\ln \varepsilon)^{-1}) \varepsilon^{-2} V((x - y)/\varepsilon), \qquad \varepsilon > 0, \quad y \in \mathbb{R}^2, \end{aligned} \tag{5.47}$$

where now

$$(U_\varepsilon g)(x) = \varepsilon^{-1} g(x/\varepsilon), \qquad \varepsilon > 0, \quad g \in L^2(\mathbb{R}^2). \tag{5.48}$$

Then the resolvent of $H_{\varepsilon,y}$ can be written as (cf. (1.2.16))

$$(H_{\varepsilon,y} - k^2)^{-1} = G_k - \lambda((\ln \varepsilon)^{-1}) A_\varepsilon(k)[1 + B_\varepsilon(k)]^{-1} C_\varepsilon(k), \qquad k^2 \in \rho(H_{\varepsilon,y}),$$
$$\operatorname{Im} k > 0, \tag{5.49}$$

where $A_\varepsilon(k)$, $B_\varepsilon(k)$, $C_\varepsilon(k)$, $\varepsilon > 0$, are Hilbert–Schmidt operators with integral kernels

$$A_\varepsilon(k, x, x') = G_k(x - y - \varepsilon x')v(x'), \qquad \operatorname{Im} k > 0, \tag{5.50}$$

$$B_\varepsilon(k, x, x') = \lambda((\ln \varepsilon)^{-1}) u(x) G_{\varepsilon k}(x - x') v(x'), \qquad \operatorname{Im} k \geq 0, \quad k \neq 0, \tag{5.51}$$

$$C_\varepsilon(k, x, x') = u(x) G_k(\varepsilon x + y - x'), \qquad \operatorname{Im} k > 0. \tag{5.52}$$

If we introduce rank-one operators $A(k)$, $C(k)$ with integral kernels

$$A(k, x, x') = G_k(x - y)v(x'), \qquad \operatorname{Im} k > 0, \tag{5.53}$$

$$C(k, x, x') = u(x) G_k(y - x'), \qquad \operatorname{Im} k > 0, \tag{5.54}$$

then as in Lemma 1.2.2

$$\lim_{\varepsilon \downarrow 0} \|A_\varepsilon(k) - A(k)\|_2 = 0, \qquad \lim_{\varepsilon \downarrow 0} \|C_\varepsilon(k) - C(k)\|_2 = 0. \tag{5.55}$$

Up to now there is no difference to our three-dimensional treatment. Due to the logarithmic singularity in $B_\varepsilon(k)$ near $k = 0$, the analysis of $B_\varepsilon(k)$ needs some care. First, we note that by the mean-value theorem (cf. (1.2.43))

$$\begin{aligned} B_\varepsilon(k) = &-(2\pi)^{-1} \lambda_1 (v, \cdot) u \\ &- (2\pi \ln \varepsilon)^{-1} \{[\lambda_1(-\Psi(1) + \ln(k/2i)) + \lambda_2](v, \cdot)u + \lambda_1 C\} + o((\ln \varepsilon)^{-1}), \end{aligned} \tag{5.56}$$

where C is a Hilbert–Schmidt operator in $L^2(\mathbb{R}^2)$ with integral kernel

$$C(x, x') = u(x) \ln|x - x'| v(x'), \qquad x \neq x', \tag{5.57}$$

and the expansion (5.56) is valid in Hilbert–Schmidt norm (the coefficients in (5.56) follow from (5.45) and the expansion of $(i/4)H_0^{(1)}(\varepsilon k|x - x'|)$ [1]). Now we have to distinguish several cases. Applying formula (1.3.47) we get:

(a) If $\lambda_1 = 0$, then, as $\varepsilon \downarrow 0$,

$$[1 + B_\varepsilon(k)]^{-1} = 1 + O((\ln \varepsilon)^{-1}). \tag{5.58}$$

(b) If $(v, u) = 0$, then $(v, \cdot)u$ is nilpotent and hence

$$[1 + B_\varepsilon(k)]^{-1} = 1 + (2\pi)^{-1}\lambda_1(v, \cdot)u + O((\ln \varepsilon)^{-1}) \tag{5.59}$$

as $\varepsilon \downarrow 0$.

(c) If $(v, u) \neq 0$ and $\lambda_1 \neq 2\pi/(v, u)$, then, as $\varepsilon \downarrow 0$,

$$[1 + B_\varepsilon(k)]^{-1} = 1 + (\lambda_1/2\pi)[1 - (\lambda_1(v, u)/2\pi)]^{-1}(v, \cdot)u + O((\ln \varepsilon)^{-1}). \tag{5.60}$$

(d) If $(v, u) \neq 0$ and $\lambda_1 = 2\pi/(v, u)$, then, as $\varepsilon \downarrow 0$,

$$\begin{aligned}[1 + B_\varepsilon(k)]^{-1} = {} & -2\pi (\ln \varepsilon)\{2\pi(v, u)[-\Psi(1) + \ln(k/2i)] + \lambda_2(v, u)^2 \\ & + (2\pi(v, Cu)/(v, u))\}(v, \cdot)u + O(1).\end{aligned} \tag{5.61}$$

Thus we obtain

Theorem 5.5. *Let $y \in \mathbb{R}^2$ and assume that V is real-valued and $(1 + |\cdot|^{2+\delta})V$, $|V|^{1+\delta} \in L^1(\mathbb{R}^2)$ for some $\delta > 0$. Then, if $k^2 \in \rho(-\Delta_{\alpha,y})$, we get $k^2 \in \rho(H_{\varepsilon,y})$ for $\varepsilon > 0$ small enough and $H_{\varepsilon,y}$ converges to $-\Delta_{\alpha,y}$ in norm resolvent sense*

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} = (-\Delta_{\alpha,y} - k^2)^{-1}, \qquad k^2 \in \rho(-\Delta_{\alpha,y}), \quad y \in \mathbb{R}^2, \tag{5.62}$$

where α is given by

$$\alpha = \begin{cases} [\lambda_2(v, u)/(2\pi)^2] + [(v, Cu)/2\pi(v, u)^2] & \text{if } (v, u) \neq 0, \ \lambda_1 = 2\pi/(v, u), \\ \infty, & \text{otherwise.} \end{cases} \tag{5.63}$$

In particular, $H_{\varepsilon,y}$ converges in norm resolvent sense to $-\Delta$ as $\varepsilon \downarrow 0$ if $(v, u) = \int_{\mathbb{R}^2} d^2x\, V(x) = 0$ or if $\lambda_1 \neq 2\pi/(v, u)$.

PROOF. Equation (5.49) together with (5.55) and (5.58)–(5.60) proves that

$$\|(H_{\varepsilon,y} - k^2)^{-1} - G_k\| = O((\ln \varepsilon)^{-1}) \tag{5.64}$$

as $\varepsilon \downarrow 0$ in cases (a)–(c). In case (d), (5.61) shows that

$$\begin{aligned}&\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,y} - k^2)^{-1} \\ &\quad = G_k + 2\pi\{-\Psi(1) + \ln(k/2i) + [(\lambda_2(v, u)/2\pi) + ((v, Cu)/(v, u)^2)]\}^{-1} \cdot \\ &\qquad \cdot (\overline{G_k(\cdot - y)}, \cdot)G_k(\cdot - y), \qquad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0.\end{aligned} \tag{5.65}$$

■

Notes

The point interaction in two dimensions is shortly discussed in Grossmann, Høegh-Krohn, and Mebkhout [226] where its local nature has also been pointed out (cf. also [253]). The treatment based on the boundary condition in (5.10) and, in particular, the final part containing scattering theory is taken from Albeverio, Gesztesy, Høegh-Krohn, and Holden [19] (for a short summary, see also [200]). The ε-expansion described at the end is also taken from [19]. For properties of the Birman–Schwinger kernel $uG_k v$ in two dimensions we refer to [248], [298], and [435]. Scattering theory near threshold is studied in [97].

External electromagnetic fields in connection with $-\Delta_{\alpha,y}$ are discussed in [381].

PART II

POINT INTERACTIONS WITH A FINITE NUMBER OF CENTERS

CHAPTER II.1

Finitely Many Point Interactions in Three Dimensions

II.1.1 Basic Properties

The aim of this section is to give a rigorous meaning to the formal operator

$$H = -\Delta - \sum_{j=1}^{N} \mu_j \delta(\cdot - y_j), \tag{1.1.1}$$

where $y_1, \ldots, y_N$ are N distinct points in $\mathbb{R}^3$.

One possible way is to employ the techniques from Sect. I.1.1 using self-adjoint extensions of symmetric operators. Here, however, we will advocate another method which, in addition to providing new insight into why the operator (I.1.1.16) is the rigorous formulation of (1.1.1) with $N = 1$, also has a flavor of renormalization techniques used in quantum field theory.

To explain the basic idea, we start with a formal manipulation when $N = 1$. Let, therefore,

$$H = -\Delta - \mu V, \tag{1.1.2}$$

where for the moment V is an appropriate potential. Expanding the resolvent we obtain

$$\begin{aligned}(H - k^2)^{-1} &= (-\Delta - \mu V - k^2)^{-1} = (1 - \mu G_k V)^{-1} G_k \\ &= G_k + \sum_{n=1}^{\infty} (\mu G_k V)^n G_k, \qquad \operatorname{Im} k > 0.\end{aligned} \tag{1.1.3}$$

If we now formally insert $V(x) = \delta(x)$ and consider the integral kernel, we obtain

$$
\begin{aligned}
(H-k^2)^{-1}(x,x') &= G_k(x-x') + \mu G_k(x)\left[\sum_{n=0}^{\infty}(\mu G_k(0))^n\right]G_k(x') \\
&= G_k(x-x') + \mu G_k(x)[1-\mu G_k(0)]^{-1}G_k(x') \qquad (1.1.4)\\
&= G_k(x-x') + G_k(x)[\mu^{-1}-G_k(0)]^{-1}G_k(x'), \qquad \operatorname{Im} k>0,
\end{aligned}
$$

which easily follows by considering, e.g., the term $(\mu G_k V)^2 G_k$:

$$
\begin{aligned}
((\mu G_k\delta)^2 G_k f)(x) &= \mu^2 \int\!\!\int\!\!\int_{\mathbb{R}^9} d^3x_1\, d^3x_2\, d^3x'\, G_k(x-x_1)\delta(x_1)\cdot \\
&\qquad \cdot G_k(x_1-x_2)\delta(x_2)G_k(x_2-x')f(x') \\
&= \mu^2 \int_{\mathbb{R}^3} d^3x'\, G_k(x)G_k(0)G_k(x')f(x'). \qquad (1.1.5)
\end{aligned}
$$

From the explicit expression $G_k(x) = e^{ik|x|}/4\pi|x|$ (cf. (I.1.1.19)) we see that of course (1.1.5), and therefore also (1.1.4), does not make sense because $G_k(0)$ does not exist. However, we still have the possibility of choosing μ. In particular, we see that if we formally write

$$
\mu^{-1} = G_0(0) + \alpha \qquad (1.1.6)
$$

with $\alpha \in \mathbb{R}$ arbitrary and interpret $G_0(0) - G_k(0)$ as

$$
\lim_{x\to 0}[G_0(x) - G_k(x)] = \lim_{x\to 0}\frac{1-e^{ik|x|}}{4\pi|x|} = -\frac{ik}{4\pi} \qquad (1.1.7)
$$

we obtain precisely the correct expression (I.1.1.20) from Part I. We also observe that the coupling constant μ in front of the δ-function has to be zero in a "suitable way" in order to make the final expression well defined.

One way to make the above rigorous is the following:

First we introduce a formal Fourier transform of the ill-defined operator H, i.e., let

$$
\begin{aligned}
&\mathscr{F}\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \\
&(\mathscr{F}f)(p) \equiv \hat{f}(p) = \operatorname*{s-lim}_{R\to\infty}(2\pi)^{-3/2}\int_{|x|\le R} d^3x\, e^{-ixp}f(x) \qquad (1.1.8)
\end{aligned}
$$

(see, e.g., [389], Sect. IX.2) and define

$$
\hat{H} = \mathscr{F}H\mathscr{F}^{-1}, \qquad (1.1.9)
$$

where

$$
(\mathscr{F}^{-1}f)(x) \equiv \check{f}(x) = \operatorname*{s-lim}_{R\to\infty}(2\pi)^{-3/2}\int_{|p|\le R} d^3p\, e^{ipx}f(p). \qquad (1.1.10)
$$

Now the Laplacian $-\Delta$ transforms into the multiplication operator with the function p^2 (see, e.g., [389], Sect. IX.7) while we formally have

$$(\mathscr{F}\delta(\cdot - y)\mathscr{F}^{-1}\hat{f})(p) = (\mathscr{F}\delta(\cdot - y)f)(p) = (2\pi)^{-3/2}e^{-ipy}f(y)$$
$$= (2\pi)^{-3}e^{-ipy}\int_{\mathbb{R}^3} d^3q\, e^{iqy}\hat{f}(q) = (\phi_y, \hat{f})\phi_y(p), \quad (1.1.11)$$

where we abbreviated

$$\phi_y(p) = (2\pi)^{-3/2}e^{-ipy}. \quad (1.1.12)$$

Thus $\hat{H}$ can be written formally as

$$\hat{H} = p^2 - \sum_{j=1}^{N} \mu_j(\phi_{y_j}, \cdot)\phi_{y_j}. \quad (1.1.13)$$

The idea is now to introduce a momentum cut-off and make the coupling constant μ_j explicitly dependent on the cut-off. More precisely, let

$$\chi_\omega(p) = \begin{cases} 1, & |p| \le \omega, \\ 0, & |p| > \omega, \end{cases} \qquad \phi_{y_j}^\omega = \chi_\omega \phi_{y_j} \quad (1.1.14)$$

and define

$$\hat{H}^\omega = p^2 - \sum_{j=1}^{N} \mu_j(\omega)(\phi_{y_j}^\omega, \cdot)\phi_{y_j}^\omega \quad (1.1.15)$$

with an interaction given by a rank N perturbation.

It remains to choose $\mu_j(\omega)$ in such a way that $\hat{H}^\omega$ has a reasonable and nontrivial limit as we remove the cut-off, i.e., as ω tends to infinity. From Theorem B.1 we obtain that

$$(\hat{H}^\omega - k^2)^{-1} = (p^2 - k^2)^{-1} + \sum_{j,j'=1}^{N} [\Gamma_\omega(k)]_{jj'}^{-1}(\chi_\omega F_{-\bar{k},y_{j'}}, \cdot)\chi_\omega F_{k,y_j},$$
$$\operatorname{Im} k > 0, \quad \operatorname{Re} k \neq 0, \quad (1.1.16)$$

where

$$\Gamma_\omega(k) = [\mu_j^{-1}(\omega)\delta_{jj'} - (\phi_{y_j}^\omega, (p^2 - k^2)^{-1}\phi_{y_{j'}}^\omega)]_{j,j'=1}^N, \qquad \operatorname{Im} k > 0, \quad (1.1.17)$$

and

$$F_{k,y}(p) = (2\pi)^{-3/2}\frac{e^{-ipy}}{p^2 - k^2}, \qquad p \in \mathbb{R}^3, \quad \operatorname{Im} k > 0. \quad (1.1.18)$$

While the quantity

$$(\phi_{y_j}^\omega, (p^2 - k^2)^{-1}\phi_{y_{j'}}^\omega) = (2\pi)^{-3}\int_{|p|\le\omega} d^3p\, \frac{e^{ip(y_j - y_{j'})}}{p^2 - k^2}, \qquad \operatorname{Im} k > 0, \quad (1.1.19)$$

diverges as ω tends to infinity when $j = j'$, the off-diagonal elements nicely converge since

$$(2\pi)^{-3}\int_{|p|\le\omega} d^3p\, \frac{e^{ipy}}{p^2 - k^2} \xrightarrow[\omega\to\infty]{} \frac{e^{ik|y|}}{4\pi|y|} = G_k(y), \qquad \operatorname{Im} k > 0, \quad y \neq 0. \quad (1.1.20)$$

(See [389], p. 58f.) If we now choose

$$\mu_j^{-1}(\omega) = (2\pi)^{-3} \int_{|p| \le \omega} \frac{d^3p}{p^2} + \alpha_j = \frac{\omega}{2\pi^2} + \alpha_j \tag{1.1.21}$$

with $\alpha_j \in \mathbb{R}$ arbitrary, we have for $\omega \to \infty$

$$\begin{aligned} \mu_j^{-1}(\omega) - (\phi_{y_j}^{\omega}, (p^2 - k^2)^{-1}\phi_{y_j}^{\omega}) &= (2\pi)^{-3} \int_{|p| \le \omega} d^3p \left(\frac{1}{p^2} - \frac{1}{p^2 - k^2}\right) + \alpha_j \\ &\xrightarrow[\omega \to \infty]{} \alpha_j - \frac{ik}{4\pi}. \end{aligned} \tag{1.1.22}$$

A short computation shows that the rank-one operator $(\chi_\omega F_{-\bar{k},y'}, \cdot)\chi_\omega F_{k,y}$ converges in Hilbert–Schmidt norm to the operator $(F_{-\bar{k},y'}, \cdot)F_{k,y}$ as $\omega \to \infty$ when $\operatorname{Im} k > 0$, i.e.,

$$\lim_{\omega \to \infty} \|(\chi_\omega F_{-\bar{k},y'}, \cdot)\chi_\omega F_{k,y} - (F_{-\bar{k},y'}, \cdot)F_{k,y}\|_2 = 0, \qquad \operatorname{Im} k > 0. \tag{1.1.23}$$

To conclude that, for $\operatorname{Im} k > 0$ sufficiently large,

$$\begin{aligned} R(k^2) &\equiv n\text{-}\lim_{\omega \to \infty} (\hat{H}^\omega - k^2)^{-1} \\ &= (p^2 - k^2)^{-1} + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} (F_{-\bar{k},y_{j'}}, \cdot)F_{k,y_j} \end{aligned} \tag{1.1.24}$$

is the resolvent of a closed operator, it is now sufficient to prove that the limit is injective ([283], Theorem VIII.1.3). Here

$$\Gamma_{\alpha,Y}(k) = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right]_{j,j'=1}^{N}, \tag{1.1.25}$$

$$\tilde{G}_k(x) = \begin{cases} G_k(x), & x \ne 0, \\ 0, & x = 0, \end{cases} \tag{1.1.26}$$

$$\alpha = (\alpha_1, \ldots, \alpha_N), \qquad Y = (y_1, \ldots, y_N). \tag{1.1.27}$$

To this end assume $R(k^2)f = 0$ for some $f \in L^2(\mathbb{R}^3)$. Using the explicit expression for $R(k^2)$ we see that this is equivalent to

$$f(p) = (2\pi)^{-3} \sum_{j,j'=1}^{N} e^{-ipy_j} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} \int_{\mathbb{R}^3} d^3q \frac{e^{iqy_{j'}} f(q)}{q^2 - k^2}, \tag{1.1.28}$$

which cannot be in $L^2(\mathbb{R}^3)$ unless $f = 0$. We can thus write $R(k^2) = (-\hat{\Delta}_{\alpha,Y} - k^2)^{-1}$. From the explicit expression for $R(k^2)$ we see that $R(k^2)^* = R(\bar{k}^2)$ which implies that the domain $\mathscr{D}(-\hat{\Delta}_{\alpha,Y})$ is dense: Let $g \perp \mathscr{D}(-\hat{\Delta}_{\alpha,Y})$. Then $(g, R(k^2)f) = 0$ for all $f \in L^2(\mathbb{R}^3)$, hence $(R(\bar{k}^2)g, f) = 0$ for all f, implying that $g = 0$. Furthermore, $-\hat{\Delta}_{\alpha,Y} = R(k^2)^{-1} + k^2$ (which is independent of k^2 from the resolvent identity) is self-adjoint because

$$\begin{aligned} (-\hat{\Delta}_{\alpha,Y}^* - \bar{k}^2)^{-1} &= [(-\hat{\Delta}_{\alpha,Y} - k^2)^*]^{-1} \\ &= [(-\hat{\Delta}_{\alpha,Y} - k^2)^{-1}]^* \\ &= (-\hat{\Delta}_{\alpha,Y} - \bar{k}^2)^{-1}, \qquad k^2 \in \rho(-\hat{\Delta}_{\alpha,Y}). \end{aligned} \tag{1.1.29}$$

We have thus proved the following theorem.

Theorem 1.1.1. *Let $\hat{H}^{\omega}$ be the self-adjoint operator in $L^2(\mathbb{R}^3)$ given by* (1.1.15) *with*

$$\mu_j(\omega) = \left(\alpha_j + \frac{\omega}{2\pi^2}\right)^{-1}, \qquad \alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N. \tag{1.1.30}$$

Then $\hat{H}^{\omega}$ converges in norm resolvent sense to a self-adjoint operator $-\hat{\Delta}_{\alpha,Y}$, i.e.,

$$(-\hat{\Delta}_{\alpha,Y} - k^2)^{-1} = \text{n-}\lim_{\omega\to\infty} (\hat{H}^{\omega} - k^2)^{-1} \tag{1.1.31}$$

for $\operatorname{Im} k > 0$ *sufficiently large, where $-\hat{\Delta}_{\alpha,Y}$ has the resolvent*

$$(-\hat{\Delta}_{\alpha,Y} - k^2)^{-1} = (p^2 - k^2)^{-1} + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(F_{-\bar{k},y_{j'}}, \cdot)F_{k,y_j},$$
$$k^2 \in \rho(-\hat{\Delta}_{\alpha,Y}), \quad \operatorname{Im} k > 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \tag{1.1.32}$$

and where $\Gamma_{\alpha,Y}(k)$, $F_{k,y}$, and *$\tilde{G}_k$ are defined by* (1.1.25), (1.1.18), *and* (1.1.26), *respectively.*

Taking now the inverse Fourier transform we finally obtain the resolvent of the *point interaction Hamiltonian* $-\Delta_{\alpha,Y}$ with N centers, viz.

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G_k(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0. \tag{1.1.33}$$

We remark that when $N = 1$ (1.1.33) of course reduces to the operator (I.1.1.20) of Part I.

We allow $\alpha_{j_0} = \infty$ for some j_0 in the sense that $-\Delta_{\alpha,Y} = -\Delta_{\tilde{\alpha},\tilde{Y}}$ where $\tilde{\alpha}$ and $\tilde{Y}$ equal α and Y, respectively, with the j_0th component removed.

For completeness we include a theorem showing how to construct the Hamiltonian with a finite number of point interactions using self-adjoint extensions of symmetric operators. However, in contrast to the one-center case, Theorem I.1.1.1, we meet a family of operators in which the centers y_1, $\ldots$, y_N are not necessarily independent although the operators are local (cf. Appendix G).

Theorem 1.1.2. *The closed symmetric operator*

$$\dot{H}_Y = -\Delta|_{\mathscr{D}_Y}, \tag{1.1.34}$$

where $Y = \{y_1, \ldots, y_N\}$ and

$$\mathscr{D}_Y = \{\phi \in H^{2,2}(\mathbb{R}^3) | \phi(y_j) = 0, y_j \in Y, j = 1, \ldots, N\} \tag{1.1.35}$$

has deficiency indices (N, N) and the deficiency subspaces read

$$\mathscr{K}_{\pm} = \operatorname{Ran}(\dot{H}_Y \pm i)^{\perp} = [G_{\sqrt{\pm i}}(\cdot - y_1), \ldots, G_{\sqrt{\pm i}}(\cdot - y_N)],$$
$$\operatorname{Im} \sqrt{\pm i} > 0. \tag{1.1.36}$$

PROOF. Since, for $\phi \in \mathscr{D}_Y$

$$(G_{\sqrt{\pm i}}(\cdot - y_j), (\dot{H}_Y \pm i)\phi) = \phi(y_j) = 0 \tag{1.1.37}$$

we immediately infer that $[G_{\sqrt{\pm i}}(\cdot - y_1), \ldots, G_{\sqrt{\pm i}}(\cdot - y_N)] \subseteq \mathscr{K}_{\pm}$. Let $\psi_{\pm} \in \operatorname{Ran}(\dot{H}_Y \pm i)^{\perp}$ and $\phi \in \mathscr{D}(-\Delta)$. Then there exist numbers $c_1, \ldots, c_N$ independent of ϕ such that

$$(\psi_{\pm}, (-\Delta \pm i)\phi) = \sum_{j=1}^{N} c_j^{\pm} \phi(y_j). \tag{1.1.38}$$

In fact, let

$$\tilde{\phi} = \phi - \sum_{j=1}^{N} \phi(y_j)\eta_j, \tag{1.1.39}$$

where $\eta_j \in C_0^{\infty}(\mathbb{R}^3)$, $\eta_j(y_j) = 1$, and $\operatorname{supp} \eta_j \cap \operatorname{supp} \eta_{j'} = \varnothing$, $j, j' = 1, \ldots, N$, $j \neq j'$. Then $\tilde{\phi} \in \mathscr{D}_Y$, and using $\psi_{\pm} \in \operatorname{Ran}(\dot{H}_Y \pm i)^{\perp}$ we infer that (1.1.38) is satisfied with $c_j^{\pm} = (\psi_{\pm}, (-\Delta \pm i)\eta_j)$. On the other hand, the constants $c_1^{\pm}, \ldots, c_N^{\pm}$ are uniquely determined by $\psi_{\pm}$ from the following computation: Assume also

$$(\tilde{\psi}_{\pm}, (-\Delta \pm i)\phi) = \sum_{j=1}^{N} c_j^{\pm} \phi(y_j). \tag{1.1.40}$$

Then

$$((\psi_{\pm} - \tilde{\psi}_{\pm}), (-\Delta \pm i)\phi) = 0 \tag{1.1.41}$$

for all $\phi \in \mathscr{D}(-\Delta)$, which implies that $\psi_{\pm} = \tilde{\psi}_{\pm}$.

Finally, we observe that

$$\psi_{\pm} = \sum_{j=1}^{N} c_j^{\pm} G_{\sqrt{\pm i}}(\cdot - y_j) \tag{1.1.42}$$

satisfies (1.1.38), thereby proving $\mathscr{K}_{\pm} \subseteq [G_{\sqrt{\pm i}}(\cdot - y_1), \ldots, G_{\sqrt{\pm i}}(\cdot - y_N)]$. ■

From the general theory of operator extensions it then follows that there exists an N^2-parameter family of self-adjoint extensions of $-\Delta|_{\mathscr{D}_Y}$. The resolvents of these operators are explicitly given by Krein's formula, Theorem A.3. However, we will only study the N-parameter family with resolvent given by (1.1.33).

As it is not possible to write $-\Delta_{\alpha,Y}$ in the form $-\Delta + V$ for any function V, we have to work with the resolvent (1.1.33). It is therefore worthwhile to note some more properties of the operator $-\Delta_{\alpha,Y}$.

Operators of the type $H = -\Delta + V$ where V is a multiplication operator are *local* in the sense that if $\psi = 0$ in some open domain of $\mathbb{R}^3$, then also $H\psi = 0$ in the same domain. From the nature of the point interaction it is reasonable to expect locality of $-\Delta_{\alpha,Y}$. This and an explicit characterization of the domain and action of $-\Delta_{\alpha,Y}$ is the content of the next theorem which generalizes Theorem I.1.1.3.

Theorem 1.1.3. *The domain $\mathscr{D}(-\Delta_{\alpha,Y})$, $y_j \in Y$, $-\infty < \alpha_j \leq \infty, j = 1, \ldots, N$, consists of all functions ψ of the type*

$$\psi(x) = \phi_k(x) + \sum_{j=1}^{N} a_j G_k(x - y_j), \qquad x \in \mathbb{R}^3 - Y, \tag{1.1.43}$$

where

$$a_j = \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}\phi(y_{j'}), \qquad j = 1, \ldots, N, \tag{1.1.44}$$

and $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3)$ *and* $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$. *This decomposition is unique, and with* ψ *of this form we have*

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{1.1.45}$$

Furthermore, let $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ *and assume* $\psi = 0$ *in an open set* $U \subseteq \mathbb{R}^3$. *Then* $-\Delta_{\alpha,Y}\psi = 0$ in U.

PROOF. Assume, without loss of generality, that $|\alpha_j| < \infty, j = 1, \ldots, N$. Then we have

$$\begin{aligned}\mathscr{D}(-\Delta_{\alpha,Y}) &= (-\Delta_{\alpha,Y} - k^2)^{-1}L^2(\mathbb{R}^3) = (-\Delta_{\alpha,Y} - k^2)^{-1}(-\Delta - k^2)\mathscr{D}(-\Delta) \\ &= \left\{1 + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} G_k(\cdot - y_j)(\overline{G_k(\cdot - y_{j'})}, (-\Delta - k^2)\cdot)\right\}\mathscr{D}(-\Delta), \\ &\qquad k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0, \end{aligned}\tag{1.1.46}$$

which proves (1.1.43) and (1.1.44). Let $\psi = 0$. Then

$$\phi_k(x) = -\sum_{j=1}^{N} a_j \frac{e^{ik|x-y_j|}}{4\pi|x - y_j|}.$$

But this function can only be continuous if $a_1 = \cdots = a_N = 0$ which implies uniqueness. Furthermore, we have

$$\begin{aligned}&(-\Delta_{\alpha,Y} - k^2)^{-1}(-\Delta - k^2)\phi_k \\ &= G_k(-\Delta - k^2)\phi_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G_k(\cdot - y_{j'})}, (-\Delta - k^2)\phi_k)G_k(\cdot - y_j) \\ &= \phi_k + \sum_{j=1}^{N} a_j G_k(\cdot - y_j) = \psi, \end{aligned}\tag{1.1.47}$$

which is equivalent to (1.1.45).

Finally, to prove locality, let ψ be of the form (1.1.43), and assume that $\psi = 0$ in an open set $U \subseteq \mathbb{R}^3$. Then

$$\phi_k(x) = -\sum_{j=1}^{N} a_j G_k(x - y_j), \qquad x \in U. \tag{1.1.48}$$

If $U \cap \{y_1, \ldots, y_N\} = \varnothing$, then we have $((-\Delta - k^2)G_k(\cdot - y_j))(x) = 0$ for $x \in U$ and for all $j = 1, \ldots, N$, which implies that

$$-\Delta_{\alpha,Y}\psi = k^2\psi + (-\Delta - k^2)\phi_k = -\sum_{j=1}^{N} a_j(-\Delta - k^2)G_k(\cdot - y_j) = 0 \tag{1.1.49}$$

in U. If, however, say $y_1 \in U$, we know from (1.1.48) that $a_1 = 0$ since ϕ is continuous, so again we can use the same argument on $G_k(\cdot - y_j)$ for $j = 2, \ldots, N$ (for a more general argument, see also Lemma C.2). ∎

Observe that $\mathscr{D}_Y \subseteq \mathscr{D}(-\Delta_{\alpha,Y})$ and that

$$-\Delta_{\alpha,Y}|_{\mathscr{D}_Y} = -\Delta|_{\mathscr{D}_Y}, \tag{1.1.50}$$

which proves that $-\Delta_{\alpha,Y}$ is among the self-adjoint extensions of Theorem 1.1.2.

In general, one expects Schrödinger Hamiltonians H of the above type to have no singular continuous spectrum, $\sigma_{sc}(H) = \varnothing$, and no positive embedded eigenvalues, i.e., $\sigma_P(H) \subseteq (-\infty, 0)$. This is also correct for point interactions as the next theorem shows. In addition, we show that eigenvalues and eigenfunctions can be determined explicitly up to the computation of the zeros of the determinant of an $N \times N$ matrix.

Theorem 1.1.4. *Let $y_j \in Y$, $-\infty < \alpha_j \leq \infty, j = 1, \ldots, N$. Then the essential spectrum of the operator $-\Delta_{\alpha,Y}$ is purely absolutely continuous and equals*

$$\sigma_{ess}(-\Delta_{\alpha,Y}) = \sigma_{ac}(-\Delta_{\alpha,Y}) = [0, \infty), \qquad \sigma_{sc}(-\Delta_{\alpha,Y}) = \varnothing. \tag{1.1.51}$$

Moreover,

$$\sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0) \tag{1.1.52}$$

and $-\Delta_{\alpha,Y}$ has at most N (negative) eigenvalues counting multiplicity. Let $\operatorname{Im} k > 0$. *Then*

$$k^2 \in \sigma_P(-\Delta_{\alpha,Y}) \quad \textit{iff}$$

$$\det[\Gamma_{\alpha,Y}(k)] = \det\left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right] = 0 \tag{1.1.53}$$

and the multiplicity of the eigenvalue k^2 equals the multiplicity of the eigenvalue zero of the matrix $\Gamma_{\alpha,Y}(k)$. Moreover, let $E_0 = k_0^2 < 0$ be an eigenvalue of $-\Delta_{\alpha,Y}$. Then the corresponding eigenfunctions ψ_0 are of the form

$$\psi_0(x) = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \qquad \operatorname{Im} k_0 > 0, \tag{1.1.54}$$

where $(c_1, \ldots, c_N)$ are eigenvectors with eigenvalue zero of the matrix $\Gamma_{\alpha,Y}(k_0)$. If $-\Delta_{\alpha,Y}$ has a ground state it is nondegenerate and the corresponding eigenfunction can be chosen to be strictly positive (i.e., the associated eigenvector $(c_1, \ldots, c_N)$ fulfills $c_j > 0, j = 1, \ldots, N$).

Proof. Without loss of generality we may assume $|\alpha_j| < \infty, j = 1, \ldots, N$. The statements concerning the essential, absolutely continuous, and singularly continuous spectrum all follow in the same way as in the one-center case, Theorem I.1.1.4. It is evident from the explicit expression for the resolvent that poles of the resolvent for $k^2 < 0$ can only occur when the matrix $\Gamma_{\alpha,Y}(k)$ is noninvertible, i.e., when it has zero determinant. Let $\operatorname{Re} k = 0, \operatorname{Im} k > 0$, and define $\kappa = -ik > 0$. Then the matrix $\Gamma_{\alpha,Y}(i\kappa)$ has the derivative

$$\frac{d\Gamma_{\alpha,Y}(i\kappa)}{d\kappa} = \left[\frac{1}{4\pi} e^{-\kappa|y_j - y_{j'}|}\right]_{j,j'=1}^{N}, \tag{1.1.55}$$

which is strictly positive definite (one can follow [437], Lemma 4.4). Therefore the N eigenvalues $\gamma_1(\kappa), \ldots, \gamma_N(\kappa)$ of $\Gamma_{\alpha,Y}(i\kappa)$ are all strictly increasing with respect to κ, and hence there can be at most N points $\kappa_1, \ldots, \kappa_N$ such that one of the eigenvalues $\gamma_j(\kappa)$, $j = 1, \ldots, N$, of $\Gamma_{\alpha,Y}(i\kappa)$ is zero. This proves the statement about the total number of negative eigenvalues. (This is also a consequence of the fact that $(-\Delta_{\alpha,Y} - k^2)^{-1} - G_k$, $\operatorname{Im} k^2 \neq 0$, is of rank N.)

Now let $E_0 = k_0^2$ be an eigenvalue of $-\Delta_{\alpha,Y}$ with corresponding eigenfunction ψ_0, i.e.,

$$-\Delta_{\alpha,Y}\psi_0 = E_0\psi_0, \qquad \psi_0 \in \mathscr{D}(-\Delta_{\alpha,Y}). \tag{1.1.56}$$

Then ψ_0 is of the form

$$\psi_0(x) = \phi_k(x) + \sum_{j=1}^{N} a_j G_k(x - y_j) \tag{1.1.57}$$

for some $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$, and $\phi_k \in \mathscr{D}(-\Delta)$ where a_j is given by (1.1.44). From the eigenvalue equation (1.1.56) and (1.1.45) it follows that

$$(-\Delta - k^2)\phi_k = (-\Delta_{\alpha,Y} - k^2)\psi_0 = (k_0^2 - k^2)\psi_0. \tag{1.1.58}$$

Hence

$$\phi_k = (k_0^2 - k^2)G_k\psi_0. \tag{1.1.59}$$

Inserting (1.1.57) into (1.1.59) we obtain

$$\phi_k = (k_0^2 - k^2)\left[G_k\phi_k + \sum_{j=1}^{N} a_j G_k G_k(\cdot - y_j)\right]. \tag{1.1.60}$$

From this equation it follows that

$$(-\Delta - k_0^2)\phi_k = (k_0^2 - k^2)\sum_{j=1}^{N} a_j G_k(\cdot - y_j). \tag{1.1.61}$$

If $E_0 = k_0^2 \geq 0$, then this equation has no nontrivial solutions. This can be seen as follows. By making a Fourier transform of eq. (1.1.61) we obtain

$$(p^2 - k_0^2)\hat{\phi}_k(p) = (2\pi)^{-3/2}(k_0^2 - k^2)\sum_{j=1}^{N} a_j \frac{e^{-ipy_j}}{p^2 - k^2}, \tag{1.1.62}$$

which proves that $\hat{\phi}_k$, and therefore ϕ_k, cannot be in $L^2(\mathbb{R}^3)$ unless it is identically zero. Hence $\psi_0 = 0$ (recall that $a_1 = \cdots = a_N = 0$ if $\phi_k = 0$), which proves the absence of nonnegative eigenvalues.

However, if $E_0 = k_0^2 < 0$, we can apply G_{k_0} on each side of (1.1.61). Using the resolvent equation we then obtain

$$\phi_k = \sum_{j=1}^{N} a_j[G_{k_0}(\cdot - y_j) - G_k(\cdot - y_j)], \tag{1.1.63}$$

which implies that ψ_0 has the form

$$\psi_0(x) = \sum_{j=1}^{N} a_j G_{k_0}(x - y_j). \tag{1.1.64}$$

By evaluating (1.1.63) at $x = y_j$ we find that

$$\phi(y_j) = \frac{1}{4\pi}(ik_0 - ik) + \sum_{j'=1}^{N} a_{j'}[\tilde{G}_{k_0}(y_j - y_{j'}) - \tilde{G}_k(y_j - y_{j'})], \qquad j = 1, \ldots, N, \tag{1.1.65}$$

(recall that $\tilde{G}_k(x) = G_k(x)$ if $x \neq 0$ and zero if $x = 0$) which can be written as

$$\phi(y_j) = \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k) - \Gamma_{\alpha,Y}(k_0)]_{jj'} a_{j'}, \qquad j = 1, \ldots, N. \tag{1.1.66}$$

Equation (1.1.44) is equivalent to

$$\phi(y_j) = \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'} a_{j'}, \qquad j = 1, \ldots, N, \tag{1.1.67}$$

which implies by (1.1.66) that

$$\sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k_0)]_{jj'} a_{j'} = 0, \qquad j = 1, \ldots, N. \tag{1.1.68}$$

Hence $(a_1, \ldots, a_N)$ is an eigenvector of $\Gamma_{\alpha,Y}(k_0)$ with eigenvalue zero.

On the other hand, if

$$\psi_0(x) = \sum_{j=1}^{N} a_j G_{k_0}(x - y_j), \qquad \operatorname{Im} k_0 > 0, \tag{1.1.69}$$

and $(a_1, \ldots, a_N)$ is an eigenvector of $\Gamma_{\alpha,Y}(k_0)$ with eigenvalue zero, we can prove that ψ_0 satisfies

$$\psi_0 \in \mathscr{D}(-\Delta_{\alpha,Y}), \qquad -\Delta_{\alpha,Y}\psi_0 = k_0^2\psi_0 \tag{1.1.70}$$

as follows. First, we wish to establish that $\psi_0 \in \mathscr{D}(-\Delta_{\alpha,Y})$. To this end, let

$$\phi_k = (k_0^2 - k^2) G_{k_0} \psi_0 \tag{1.1.71}$$

for some $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$. Then $\phi \in \mathscr{D}(-\Delta)$ and we have the following computation

$$\phi_k = (k_0^2 - k^2) \sum_{j=1}^{N} a_j G_k G_{k_0}(\cdot - y_j) = \sum_{j=1}^{N} a_j [G_{k_0}(\cdot - y_j) - G_k(\cdot - y_j)], \tag{1.1.72}$$

which implies that

$$\phi_k + \sum_{j=1}^{N} a_j G_k(\cdot - y_j) = \sum_{j=1}^{N} a_j G_{k_0}(\cdot - y_j) = \psi_0. \tag{1.1.73}$$

To prove that $a_j, j = 1, \ldots, N$, satisfy (1.1.44) we evaluate (1.1.72) at y_j. Then

$$\begin{aligned}
\phi_k(y_j) &= \frac{1}{4\pi}(ik_0 - ik) + \sum_{j'=1}^{N} a_{j'}[\tilde{G}_{k_0}(y_j - y_{j'}) - \tilde{G}_k(y_j - y_{j'})] \\
&= \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k) - \Gamma_{\alpha,Y}(k_0)]_{jj'} a_{j'} \\
&= \sum_{j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'} a_{j'}, \qquad j = 1, \ldots, N,
\end{aligned} \tag{1.1.74}$$

which proves (1.1.44), and hence $\psi_0 \in \mathscr{D}(-\Delta_{\alpha,Y})$. Finally, we observe that

$$-\Delta_{\alpha,Y}\psi_0 = (-\Delta - k^2)\phi_k + k^2\psi_0 = (k_0^2 - k^2)\psi_0 + k^2\psi_0 = k_0^2\psi_0. \tag{1.1.75}$$

The assertions about the ground state follow from the monotone increase of all eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$ for $\kappa > 0$ and the fact that $\Gamma_{\alpha,Y}(i\kappa)$ generates a positivity preserving semigroup $e^{-t\Gamma_{\alpha,Y}(i\kappa)}$, $t \geq 0$, $\kappa \in \mathbb{R}$, in $\mathbb{C}^N$ since all off-diagonal elements in $\Gamma_{\alpha,Y}(i\kappa)$ are negative ([391], p. 210). Thus the smallest eigenvalue of $\Gamma_{\alpha,Y}(i\kappa)$ is nondegenerate and we may choose a corresponding nonnegative eigenvector $(c_1, \ldots, c_N)$, $c_j \geq 0, j = 1, \ldots, N$. Since $c_{j_0} = 0$ for some j_0 would imply $\alpha_{j_0} = \infty$ we actually infer $c_j > 0, j = 1, \ldots, N$ (cf. also the discussion in Appendix F). ∎

Before we give an example to illustrate the results in a simple case, we note the following elementary result.

Proposition 1.1.5. *Let $N(k^2, \alpha_1, \ldots, \alpha_N)$ denote the number of eigenvalues (counting multiplicities) of $-\Delta_{\alpha,Y}$ less than or equal to $k^2 < 0$. Then*

$$N(k^2, \bar{\alpha}, \ldots, \bar{\alpha}) \leq N(k^2, \alpha_1, \ldots, \alpha_N) \leq N(k^2, \underline{\alpha}, \ldots, \underline{\alpha}), \tag{1.1.76}$$

where

$$\bar{\alpha} = \max_{1 \leq j \leq N} (\alpha_j), \qquad \underline{\alpha} = \min_{1 \leq j \leq N} (\alpha_j). \tag{1.1.77}$$

PROOF. Observe from (1.1.25) that the eigenvalues of $\Gamma_{\alpha,Y}(k)$, $\operatorname{Im} k > 0$, $\operatorname{Re} k = 0$, are increasing in each of the components α_j of α, which proves (1.1.76). ∎

One virtue of point interactions is, as we have already seen in the one-center case, that eigenvalues and resonances can be treated on an equal footing. We define resonances of $-\Delta_{\alpha,Y}$ as follows. $k_0 \in \mathbb{C}$, $\operatorname{Im} k_0 \leq 0$, is a resonance of $-\Delta_{\alpha,Y}$ iff

$$\det[\Gamma_{\alpha,Y}(k_0)] = \det\left[\left(\alpha_j - \frac{ik_0}{4\pi}\right)\delta_{jj'} - \tilde{G}_{k_0}(y_j - y_{j'})\right] = 0.$$

The multiplicity of the resonance k_0 equals the multiplicity of the zero of $\det[\Gamma_{\alpha,Y}(k)]$ at $k = k_0$.

We end this section with an example illustrating some of the ideas in this chapter, namely the study of the two-center problem with equal strength, i.e., $N = 2$, $\alpha_1 = \alpha_2 = \alpha$, in eq. (1.1.33).

The eigenvalue/resonance equation is (with $L = |y_1 - y_2|$)

$$\det\begin{bmatrix} \alpha - \dfrac{ik}{4\pi} & G_k(L) \\ G_k(L) & \alpha - \dfrac{ik}{4\pi} \end{bmatrix} = \left(\alpha - \frac{ik}{4\pi}\right)^2 - G_k(L)^2 = 0, \tag{1.1.78}$$

i.e.,

$$4\pi\alpha L - ikL = \pm e^{ikL}. \tag{1.1.79}$$

Now let $Lk = x + iy$. Separating the real and imaginary part we obtain the two equations

$$\begin{aligned} 4\pi\alpha L + y &= \pm e^{-y}\cos x, \\ -x &= \pm e^{-y}\sin x. \end{aligned} \tag{1.1.80}$$

Eigenvalues correspond to $x = 0$ and $y > 0$, i.e.,

$$y = \pm e^{-y} - 4\pi\alpha L. \tag{1.1.81}$$

From Figure 2 we see that if $4\pi\alpha L < -1$ we have two simple eigenvalues, if $1 > 4\pi\alpha L \geq -1$ we have one simple eigenvalue, and finally, if $4\pi\alpha L \geq 1$ there are no eigenvalues.

To study the resonances we have to look for solutions of (1.1.80) with $y < 0$ and x arbitrary. First, we observe that if (x, y) is a solution of (1.1.80) then $(-x, y)$ is also a solution, i.e., we have a reflection symmetry with respect to the imaginary axis. So we only have to study what happens when $x > 0$. We can rewrite (1.1.80) as

$$y = \ln \left| \frac{\sin x}{x} \right| \tag{1.1.82}$$

and

$$y = -x \cot x - 4\pi\alpha L. \tag{1.1.83}$$

Let ϕ be the monotone decreasing function on $((2n - 1)\pi, 2n\pi)$

$$\phi(x) = \ln \left| \frac{\sin x}{x} \right| + x \cot x + 4\pi\alpha L. \tag{1.1.84}$$

As $x \downarrow (2n - 1)\pi$, $\phi(x) \to +\infty$, and as $x \uparrow 2n\pi$, $\phi(x) \to -\infty$, $n \in \mathbb{N}$, which implies that for each interval $((2n - 1)\pi, 2n\pi)$, $n \in \mathbb{N}$, there is precisely one simple resonance k_n such that $\operatorname{Re} k_n \in ((2n - 1)(\pi/L), 2n(\pi/L))$. Similarly, there is exactly one simple resonance k_n such that $\operatorname{Re} k_n \in (2n(\pi/L), (2n + 1)(\pi/L))$. On the interval $[0, \pi)$ we have that as $x \downarrow 0$, $\phi(x) \to 1 + 4\pi\alpha L$, while as $x \uparrow \pi$, $\phi(x) \to -\infty$. Thus if $4\pi\alpha L > -1$ we have, as before, exactly one simple resonance k_1 with $\operatorname{Re} k_1 \in (0, (\pi/L))$. If $4\pi\alpha L < -1$ we have exactly one simple resonance on the negative imaginary axis, which we have already encountered in Figure 2. When α varies in $\mathbb{R}$, we see that we can always satisfy eq. (1.1.83), thus we have the resonance curves as shown in Figure 3.

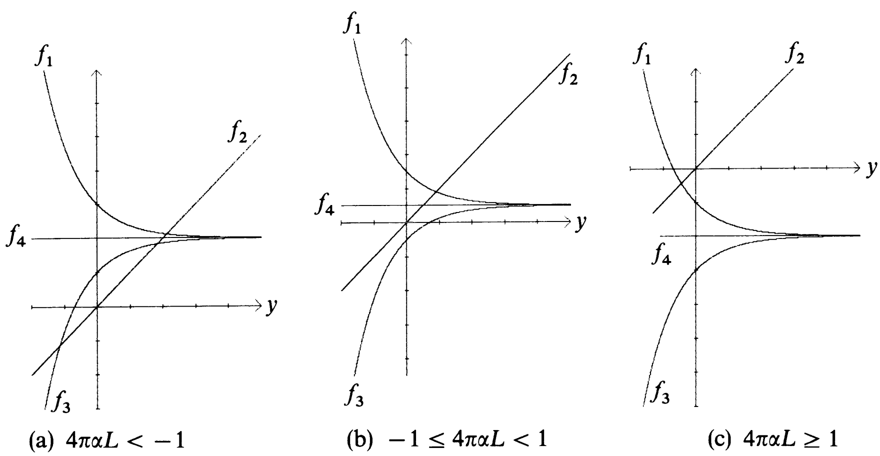


Figure 2 $f_1(y) = e^{-y} - 4\pi\alpha L$; $f_2(y) = y$; $f_3(y) = -e^{-y} - 4\pi\alpha L$; $f_4(y) = -4\pi\alpha L$.

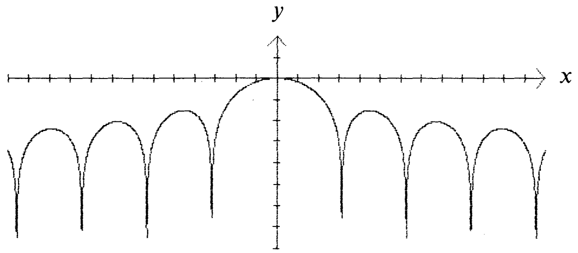


Figure 3 $y = \ln \left| \frac{\sin x}{x} \right|$.

Finally, we note that the asymptotic behavior of the resonances k_n is given by

$$k_n \approx (n + \tfrac{1}{2})\frac{\pi}{L} - \frac{i}{L}\ln[(n + \tfrac{1}{2})\pi] \qquad (1.1.85)$$

as $n \to \infty$.

We will return to this example in Sect. 1.4.

II.1.2 Approximations by Means of Local Scaled Short-Range Interactions

Having defined the point interaction Hamiltonian $-\Delta_{\alpha,Y}$, it is reasonable to ask in what sense this Hamiltonian is approximated by Hamiltonians with more realistic and less singular short-range interactions.

Let

$$H_{\varepsilon,Y} = \Delta \dotplus \varepsilon^{-2} \sum_{j=1}^{N} \lambda_j(\varepsilon) V_j((\cdot - y_j)/\varepsilon), \qquad \varepsilon > 0, \qquad (1.2.1)$$

where $V_j \in R, j = 1, \ldots, N$ (recall that the Rollnik class R consists of functions $V: \mathbb{R}^3 \to \mathbb{C}$ with $\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3y \, |V(x)| \, |V(y)| \, |x - y|^{-2} < \infty$) are real-valued and $\lambda_j(\varepsilon)$ are assumed to be real-analytic in a neighborhood of zero with

$$\lambda_j(0) = 1, \qquad j = 1, \ldots, N. \qquad (1.2.2)$$

The set $Y = \{y_1, \ldots, y_N\}$ of N distinct points $y_j \in \mathbb{R}^3, j = 1, \ldots, N$, forms the set where we want to localize the point interactions. (We will use Y to denote both the set $\{y_1, \ldots, y_N\} \subset \mathbb{R}^3$ and the n-tuple $(y_1, \ldots, y_N) \in \mathbb{R}^{3N}$ when no confusion can arise.) $H_{\varepsilon,Y}$ is well defined as a sum of quadratic forms by Appendix B.

Recall from Sect. I.1.1 the unitary scaling group U_ε in $L^2(\mathbb{R}^3)$ given by

$$(U_\varepsilon g)(x) = \varepsilon^{-3/2} g(x/\varepsilon), \qquad \varepsilon > 0, \quad g \in L^2(\mathbb{R}^3), \qquad (1.2.3)$$

which connects $H_{\varepsilon,Y}$ to the self-adjoint operator $H_Y(\varepsilon)$ defined by

$$H_Y(\varepsilon) \equiv \varepsilon^2 U_\varepsilon^{-1} H_{\varepsilon,Y} U_\varepsilon = -\Delta \dotplus \sum_{j=1}^{N} \lambda_j(\varepsilon) V_j(\cdot - \varepsilon^{-1} y_j), \qquad \varepsilon > 0. \quad (1.2.4)$$

We will also need the operators

$$H_j = -\Delta \dotplus V_j, \qquad j = 1, \ldots, N. \tag{1.2.5}$$

Then we have the following theorem.

Theorem 1.2.1. *Let V_j: $\mathbb{R}^3 \to \mathbb{R}$ fulfill $(1 + |\cdot|)^2 V_j \in R \cap L^1(\mathbb{R}^3)$, $j = 1, \ldots, N$. Assume, in addition, that $\lambda_j'(0) \neq 0$ if $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV *for some $j = 1, \ldots, N$. Then the operator $H_{\varepsilon, Y}$ defined by* (1.2.1) *converges in strong resolvent sense to the operator $-\Delta_{\alpha, Y}$ defined by* (1.1.33) *where $\alpha = (\alpha_1, \ldots, \alpha_N)$ is given by*

$$\alpha_j = \begin{cases} \infty & \text{in case I}, \\ -\lambda_j'(0)|(v_j, \phi_j)|^{-2} & \text{in case II}, \\ \infty & \text{in case III}, \\ -\lambda_j'(0)\left\{\sum_{l=1}^{N_j} |(v_j, \phi_{jl})|^2\right\}^{-1} & \text{in case IV}. \end{cases} \tag{1.2.6}$$

Here ϕ_j (resp. ϕ_{jl}, $l = 1, \ldots, N_j$) denote eigenvectors of $u_j G_0 v_j$ to the eigenvalue -1 with (cf. Sect. I.1.2)

$$(\tilde{\phi}_j, \phi_j) = -1, \qquad (\tilde{\phi}_{jl}, \phi_{jl'}) = -\delta_{ll'}, \qquad l, l' = 1, \ldots, N_j, \quad j = 1, \ldots, N. \tag{1.2.7}$$

Remark. As remarked earlier, $\alpha_{j_0} = \infty$ for some j_0 means that the point (α_{j_0}, y_{j_0}) should be removed from the definition of $-\Delta_{\alpha, Y}$, i.e., we obtain $-\Delta_{\tilde{\alpha}, \tilde{Y}}$ where $\tilde{\alpha} = (\alpha_1, \ldots, \alpha_{j_0 - 1}, \alpha_{j_0 + 1}, \ldots, \alpha_N)$ and $\tilde{Y} = (y_1, \ldots, y_{j_0 - 1}, y_{j_0 + 1}, \ldots, y_N)$, etc.

PROOF. The proof of the theorem is divided into two lemmas.

Lemma 1.2.2. *The resolvent of $H_{\varepsilon, Y}$ reads*

$$(H_{\varepsilon, Y} - k^2)^{-1} = G_k - \varepsilon \sum_{j, j'=1}^{N} A_{\varepsilon, j}(k)[1 + B_\varepsilon(k)]_{jj'}^{-1} C_{\varepsilon, j'}(k),$$

$$k^2 \in \rho(H_{\varepsilon, Y}), \quad \operatorname{Im} k > 0, \quad \varepsilon > 0, \tag{1.2.8}$$

where $A_{\varepsilon, j}(k)$, $B_\varepsilon(k) = [B_{\varepsilon, jj'}(k)]_{j, j'=1}^N$, and $C_{\varepsilon, j}(k)$ are Hilbert–Schmidt operators with integral kernels

$$A_{\varepsilon, j}(k)(x, x') = \lambda_j(\varepsilon) G_k(x - y_j - \varepsilon x') v_j(x'),$$

$$B_{\varepsilon, jj'}(k)(x, x') = \begin{cases} \lambda_j(\varepsilon) u_j(x) G_{\varepsilon k}(x - x') v_j(x'), & j = j', \\ \varepsilon \lambda_j(\varepsilon) u_j(x) G_k(\varepsilon(x - x') + y_j - y_{j'}) v_{j'}(x'), & j \neq j', \end{cases} \tag{1.2.9}$$

$$C_{\varepsilon, j}(k)(x, x') = u_j(x) G_k(\varepsilon x + y_j - x'); \quad j, j' = 1, \ldots, N, \quad \operatorname{Im} k \geq 0, \quad \varepsilon \geq 0.$$

PROOF OF LEMMA 1.2.2. Using Theorem B.1 we have

$$[H_Y(\varepsilon) - (\varepsilon k)^2]^{-1} = G_{\varepsilon k} - \sum_{j, j'=1}^{N} \lambda_j(\varepsilon) G_{\varepsilon k} \tilde{v}_j [1 + \tilde{B}_\varepsilon(\varepsilon k)]_{jj'}^{-1} \tilde{u}_{j'} G_{\varepsilon k},$$

$$(\varepsilon k)^2 \in \rho(H_Y(\varepsilon)), \quad \operatorname{Im} k > 0, \tag{1.2.10}$$

where

$$\tilde{v}_j(x) = v_j(x - \varepsilon^{-1}y_j), \qquad \tilde{u}_j(x) = u_j(x - \varepsilon^{-1}y_j), \qquad \varepsilon > 0, \quad j = 1, \ldots, N, \tag{1.2.11}$$

and

$$\tilde{B}_\varepsilon(\varepsilon k) = [\tilde{B}_\varepsilon(\varepsilon k)_{jj'}]_{j,j'=1}^N = [\lambda_j(\varepsilon)\tilde{u}_j G_{\varepsilon k}\tilde{v}_{j'}]_{j,j'=1}^N. \tag{1.2.12}$$

In addition to the scaling operator U_ε given by (1.2.3) we also need the unitary translation operators

$$T_y\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \qquad (T_y g)(x) = g(x + y), \qquad g \in L^2(\mathbb{R}^3), \quad y \in \mathbb{R}^3. \tag{1.2.13}$$

Recall that

$$\varepsilon^2 U_\varepsilon G_{\varepsilon k} U_\varepsilon^{-1} = G_k, \qquad \varepsilon > 0, \quad \operatorname{Im} k > 0. \tag{1.2.14}$$

With all this we can compute the resolvent of $H_{\varepsilon, Y}$.

$$\begin{aligned}
&(H_{\varepsilon,Y} - k^2)^{-1}\\
&\quad = \varepsilon^2 U_\varepsilon[H_Y(\varepsilon) - (\varepsilon k)^2]^{-1}U_\varepsilon^{-1}\\
&\quad = G_k - \varepsilon^{-2}\sum_{j,j'=1}^N \lambda_j(\varepsilon)G_k U_\varepsilon \tilde{v}_j[1 + \tilde{B}_\varepsilon(\varepsilon k)]_{jj'}^{-1}\tilde{u}_{j'}U_\varepsilon^{-1}G_k\\
&\quad = G_k - \varepsilon^{-2}\sum_{j,j'=1}^N \lambda_j(\varepsilon)G_k U_\varepsilon \tilde{v}_j T_{y_j/\varepsilon}^{-1}T_{y_j/\varepsilon}[1 + \tilde{B}_\varepsilon(\varepsilon k)]_{jj'}^{-1}T_{y_{j'}/\varepsilon}^{-1}T_{y_{j'}/\varepsilon}\tilde{u}_{j'}U_\varepsilon^{-1}G_k\\
&\quad = G_k - \varepsilon\sum_{j,j'=1}^N A_{\varepsilon,j}(k)[1 + B_\varepsilon(k)]_{jj'}^{-1}C_{\varepsilon,j'}(k), \qquad k^2 \in \rho(H_{\varepsilon,Y}), \quad \operatorname{Im} k > 0.
\end{aligned}\tag{1.2.15}$$

■

As in the one-center case the problem is now reduced to the study of the limit of the operators $A_{\varepsilon,j}(k)$, $[1 + B_\varepsilon(k)]_{jj'}^{-1}$, $C_{\varepsilon,j'}(k)$ as $\varepsilon \downarrow 0$. As in Lemma I.1.2.2 we obtain convergence of

$$\begin{aligned}
&A_{\varepsilon,j}(k) \xrightarrow[\varepsilon\downarrow 0]{} A_{0,j}(k) = (v_j, \cdot)G_k(\cdot - y_j),\\
&C_{\varepsilon,j}(k) \xrightarrow[\varepsilon\downarrow 0]{} C_{0,j}(k) = (\overline{G_k(\cdot - y_j)}, \cdot)u_j, \qquad j = 1, \ldots, N, \quad \operatorname{Im} k > 0,
\end{aligned}\tag{1.2.16}$$

in Hilbert–Schmidt norm where we observe that $A_{0,j}(k)$ and $C_{0,j}(k)$, $j = 1, \ldots, N$, are rank-one operators.

The limit of $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ is much more delicate. We split the operator $B_\varepsilon \equiv [B_{\varepsilon,jj'}(k)]_{j,j'=1}^N$ in the diagonal and off-diagonal elements, i.e.,

$$B_\varepsilon = D_\varepsilon + \varepsilon E_\varepsilon, \tag{1.2.17}$$

where $D_\varepsilon = [D_{\varepsilon,jj'}]_{j,j'=1}^N$ and $E_\varepsilon = [E_{\varepsilon,jj'}]_{j,j'=1}^N$ have integral kernels

$$\begin{aligned}
&D_{\varepsilon,jj'}(x, x') = \delta_{jj'}\lambda_j(\varepsilon)u_j(x)G_{\varepsilon k}(x - x')v_j(x'),\\
&E_{\varepsilon,jj'}(x, x') = (1 - \delta_{jj'})\lambda_j(\varepsilon)u_j(x)G_k(\varepsilon(x - x') + y_j - y_{j'})v_{j'}(x'), \qquad \varepsilon \geq 0.
\end{aligned}\tag{1.2.18}$$

From this decomposition it follows that

$$\varepsilon[1 + B_\varepsilon]^{-1} = \varepsilon[1 + D_\varepsilon + \varepsilon E_\varepsilon]^{-1} = \{1 + \varepsilon[1 + D_\varepsilon]^{-1}E_\varepsilon\}^{-1}\varepsilon[1 + D_\varepsilon]^{-1}, \tag{1.2.19}$$

which implies that we have to find the limit of $\varepsilon[1 + D_\varepsilon]^{-1}$ and E_ε as ε tends to zero. Now the limit of the operator $\varepsilon[1 + D_\varepsilon]^{-1}$ corresponds to the limit of the operator

$\varepsilon[1 + B_\varepsilon(k)]^{-1}$ in the one-center case which was computed in Lemma I.1.2.4., i.e.,

$$F_{jj} \equiv \underset{\varepsilon \downarrow 0}{\text{n-lim}}\, \varepsilon(1 + D_{\varepsilon,jj})^{-1} = \begin{cases} 0 & \text{in case I,} \\ [(ik/4\pi)|(v_j, \phi_j)|^2 + \lambda_j'(0)]^{-1}(\tilde{\phi}_j, \cdot)\phi_j & \text{in case II,} \\ -[\lambda_j'(0)]^{-1} \sum_{l=1}^{N_j} (\tilde{\phi}_{jl}, \cdot)\phi_{jl} & \text{in case III,} \\ \sum_{l,l'=1}^{N_j} [(4\pi)^{-1} ik(\tilde{\phi}_{jl}, u_j)(v_j, \phi_{jl'}) & \\ \quad + \lambda_j'(0)\delta_{ll'}]^{-1}(\tilde{\phi}_{jl'}, \cdot)\phi_{jl} & \text{in case IV,} \end{cases} \tag{1.2.20}$$

where $[\cdot]^{-1}$ denotes the inverse matrix in case IV.

So far we only needed the conditions $V_j \in R$ and $(1 + |\cdot|)V_j \in L^1(\mathbb{R}^3)$, $\lambda_j'(0) \neq 0$ in cases III and IV, $j = 1, \ldots, N$, but to control the limit of E_ε we use $(1 + |\cdot|)^2 V_j \in R \cap L^1(\mathbb{R}^3)$.

Lemma 1.2.3. *If $V_j\colon \mathbb{R}^3 \to \mathbb{R}$ satisfies $(1 + |\cdot|)^2 V_j \in R \cap L^1(\mathbb{R}^3)$, $j = 1, \ldots, N$, then $\|E_\varepsilon\|$ is uniformly bounded and*

$$\underset{\varepsilon \to 0}{\text{s-lim}}\, E_\varepsilon = E_0 = [(1 - \delta_{jj'})G_k(y_j - y_{j'})(v_{j'}, \cdot)u_j]_{j,j'=1}^N \qquad \operatorname{Im} k > 0. \tag{1.2.21}$$

Proof of Lemma 1.2.3. To simplify the notation we assume $\lambda_j(\varepsilon) \equiv 1$. First, we show that $\|E_\varepsilon\|$ is uniformly bounded by estimating $\|E_{\varepsilon,jj'}\|_2$, $j \neq j'$ (see [250]) as follows

$$\|E_{\varepsilon,jj'} - E_{0,jj'}\|_2^2 \leq \frac{1}{4\pi^2|y_j - y_{j'}|^2}\{\|(1 + |\cdot|^2)V_j\|_R \|(1 + |\cdot|^2)V_{j'}\|_R + 2\|V_j\|_{L^1(\mathbb{R}^3)}\|V_{j'}\|_{L^1(\mathbb{R}^3)}\}. \tag{1.2.22}$$

Let $f \in C_0^\infty(\mathbb{R}^3)$. Using the fact that f has compact support and that $(1 + |\cdot|)V_j \in L^1(\mathbb{R}^3)$, one can prove (see [250], Lemma 2.4) that

$$\|(E_{\varepsilon,jj'} - E_{0,jj'})f\| \to 0 \quad \text{as } \varepsilon \downarrow 0, \qquad j, j' = 1, \ldots, N, \quad \operatorname{Im} k > 0. \tag{1.2.23}$$

The uniform bound on $\|E_\varepsilon\|$ then completes the proof. ■

Using the resolvent identity we now obtain

$$\{1 + \varepsilon[1 + D_\varepsilon]^{-1}E_\varepsilon\}^{-1} = [1 + FE_0]^{-1} + \{1 + \varepsilon[1 + D_\varepsilon]^{-1}E_\varepsilon\}^{-1} \cdot \cdot\{\varepsilon[1 + D_\varepsilon]^{-1}E_\varepsilon - FE_0\}[1 + FE_0]^{-1} \xrightarrow[\varepsilon \downarrow 0]{s} [1 + \mathrm{F}\mathrm{E}_0]^{-1}. \tag{1.2.24}$$

Together with (1.2.16) and (1.2.20) this implies that

$$\varepsilon[1 + B_\varepsilon]^{-1} \xrightarrow[\varepsilon \downarrow 0]{s} [1 + FE_0]^{-1}F, \qquad \operatorname{Im} k > 0. \tag{1.2.25}$$

We are now in possession of the limits of all operators involved in $(H_{\varepsilon,Y} - k^2)^{-1}$. By a tedious but straightforward calculation [247] we obtain the result stated in the theorem, viz.

$$\underset{\varepsilon \downarrow 0}{\text{s-lim}}\, (H_{\varepsilon,Y} - k^2)^{-1} = G_k - \sum_{j,j'=1}^N A_{0,j}(k)[[1 + FE_0]^{-1}F]_{jj'}C_{0,j'}(k)$$
$$= G_k + \sum_{j,j'=1}^N [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j), \tag{1.2.26}$$

where $\alpha = (\alpha_1, \ldots, \alpha_N)$ is given in (1.2.6). ■

We can also obtain norm resolvent convergence in the N-center case, but then we need stronger decay on the potential.

Theorem 1.2.4. *Let $V_j \in R$ be real-valued and* supp V_j *compact, $j = 1, \ldots, N$. Assume, in addition, that $\lambda_j'(0) \neq 0$ if H_j is in case* III *or* IV *for some $j = 1, \ldots, N$. Then $H_{\varepsilon, Y}$ converges in norm resolvent sense to $-\Delta_{\alpha, Y}$ where α is given by* (1.2.6).

PROOF. As Rollnik functions with compact support are in $L^1(\mathbb{R}^3)$ ([434], Theorem I.7) the only thing we have to prove, when compared with the preceding theorem, is that

$$\|E_\varepsilon - E_0\| \to 0 \quad \text{as } \varepsilon \downarrow 0. \tag{1.2.27}$$

Since the potentials have bounded support we can assume that the variables x, x' in the definition (1.2.18) of E_ε satisfy $|x|, |x'| < c$, when we estimate the Hilbert–Schmidt norm of $E_\varepsilon - E_0$ which implies that $|\varepsilon(x - x') + y_j - y_{j'}| \geq |y_j - y_{j'}| - 2\varepsilon c > 0$ for all ε sufficiently small. Using the dominated convergence theorem (1.2.27) readily follows. ■

II.1.3 Convergence of Eigenvalues and Resonances

Using the convergence results from the previous section we now deduce results concerning the convergence of eigenvalues and resonances.

Theorem 1.3.1. *Let $V_j \in R$ be real-valued,* supp V_j *compact, $j = 1, \ldots, N$, and suppose* (I.1.2.84). *Moreover, if $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV *for some j we assume, in addition, $\lambda_j'(0) \neq 0$. Assume that k_0^2,* $\operatorname{Im} k_0 > 0$, *is a negative eigenvalue of $-\Delta_{\alpha, Y}$ (the norm resolvent limit of $H_{\varepsilon, Y}$ as $\varepsilon \downarrow 0$) with multiplicity M. Then there exist functions h_l, $l = 1, \ldots, m$, analytic near the origin, $h_l(0) = 0$, and integers $m_l \in \{1, 2\}$, $l = 1, \ldots, m$, such that*

$$\begin{aligned} k_{l,\varepsilon}^2 &= k_0^2 + h_l(\varepsilon^{1/m_l}) \\ &= k_0^2 + \sum_{r=1}^{\infty} a_{l,r} \varepsilon^{r/m_l}, \qquad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M, \end{aligned} \tag{1.3.1}$$

are all the eigenvalues of $H_{\varepsilon, Y}$ near k_0^2 for $\varepsilon > 0$ sufficiently small. If $m_l = 2$ for some l, both square roots should be used such that the total multiplicity of all eigenvalues of $H_{\varepsilon, Y}$ near k_0^2 is exactly M. Furthermore,

$$k_{l,\varepsilon} = k_0 + \varepsilon^{1/m_l} k_l^1 + o(\varepsilon^{1/m_l}), \tag{1.3.2}$$

where $k_l^1 = k_1$ is a solution of (1.3.33) *if $m_l = 1$ and of* (1.3.36) *if $m_l = 2$.*

Remark. Since cases I and III do not give rise to any interaction in the limit $\varepsilon \downarrow 0$, we have implicitly assumed in the above that $H_j = -\Delta \dotplus V_j$ is in case II or IV for at least one j.

PROOF. From the analysis of Appendix B we know that $k_\varepsilon^2 < 0$ is an eigenvalue of $H_{\varepsilon,Y}$ iff -1 is an eigenvalue of $B_\varepsilon(k_\varepsilon)$, Im $k_\varepsilon > 0$, where $B_\varepsilon(k_\varepsilon)$ is given by (1.2.9), and hence iff

$$\det{}_2[1 + B_\varepsilon(k_\varepsilon)] = 0. \tag{1.3.3}$$

But since the operator $B_\varepsilon(k)$ does not depend on k when $\varepsilon = 0$, we cannot use the implicit function theorem in (1.3.3) directly. Instead we expand the operator $B_\varepsilon(k)$ in norm in powers of ε, viz.

$$B_\varepsilon(k) = B + \varepsilon\hat{B}(k) + o(\varepsilon), \tag{1.3.4}$$

where

$$\begin{aligned} B &= [\delta_{jj'}u_j G_0 v_j]_{j,j'=1}^N, \\ \hat{B}(k) &= \left\{\left[\lambda_j'(0)u_j G_0 v_j + \frac{ik}{4\pi}(v_j, \cdot)u_j\right]\delta_{jj'} + \tilde{G}_k(y_j - y_{j'})(v_{j'}, \cdot)u_j\right\}_{j,j'=1}^N. \end{aligned} \tag{1.3.5}$$

We know that $\operatorname{Ker}(1 + B) = \{\Phi \in \mathscr{H} \mid (1 + B)\Phi = 0\}$, with $\mathscr{H} = \oplus_{j=1}^N L^2(\mathbb{R}^3)$, consists of vectors of the form

$$\Phi = (\Phi_1, \ldots, \Phi_N), \tag{1.3.6}$$

where

$$\Phi_j = \begin{cases} 0 & \text{if } H_j = -\Delta \dotplus V_j \text{ is in case I,} \\ a_j\phi_j & \text{if } H_j = -\Delta \dotplus V_j \text{ is in case II,} \\ \sum_{l=1}^{N_j} a_{jl}\phi_{jl} & \text{if } H_j = -\Delta \dotplus V_j \text{ is in case III or IV;} \quad j = 1, \ldots, N. \end{cases} \tag{1.3.7}$$

We now want to decompose the Hilbert space $\mathscr{H}$ as follows. Let $\tilde{P} = [\delta_{jj'}P_j]$ be the projection

$$P_j = \begin{cases} 0 & \text{in case I,} \\ -(\tilde{\phi}_j, \cdot)\phi_j & \text{in case II,} \\ -\sum_{l=1}^{N_j} (\tilde{\phi}_{jl}, \cdot)\phi_{jl} & \text{in case III or IV;} \quad j = 1, \ldots, N, \end{cases} \tag{1.3.8}$$

and let

$$\begin{aligned} \tilde{\mathscr{H}} &= \operatorname{Ker}(1 + B) = \operatorname{Ran} \tilde{P}, \\ \mathscr{H}_2 &= \operatorname{Ran}(1 + B). \end{aligned} \tag{1.3.9}$$

Using

$$\operatorname{Ker} \tilde{P} = \operatorname{Ker}(1 + B^*)^\perp \tag{1.3.10}$$

and the Fredholm alternative ([494], p. 136) we infer that

$$\mathscr{H}_2 = \operatorname{Ker} \tilde{P}. \tag{1.3.11}$$

Thus $\mathscr{H}$ can be written as a direct sum

$$\mathscr{H} = \tilde{\mathscr{H}} \dotplus \mathscr{H}_2. \tag{1.3.12}$$

The space $\tilde{\mathscr{H}}$ so far consists of all eigenvectors of B with eigenvalue -1, while the limit operator $-\Delta_{\alpha,Y}$ is only affected by the eigenvector in case II and the one eigenvector in case IV which gives rise to the zero-energy resonance (with our convention this is ϕ_{j1} in case IV, cf. (I.1.2.84)). Because of this we put all these eigenvectors in a space $\mathscr{H}_0$ and let $\mathscr{H}_1$ be the complement, thus

$$\tilde{\mathscr{H}} = \mathscr{H}_0 \dot{+} \mathscr{H}_1. \tag{1.3.13}$$

Define

$$\begin{aligned} B_{00} &= P_0 B P_0, & B_{10} &= (1 - P_0) B P_0, \\ B_{01} &= P_0 B (1 - P_0), & B_{11} &= (1 - P_0) B (1 - P_0) \end{aligned} \tag{1.3.14}$$

and similarly for $\hat{B}(k)$ and $o(\varepsilon)$. Here P_0 is the part of $\tilde{P}$ projecting onto $\mathscr{H}_0$. Then $B_{00} = -P_0$ and $B_{01} = B_{10} = 0$ which implies that $B_\varepsilon(k)$ can be written as

$$B_\varepsilon(k) = \begin{bmatrix} -1 + \varepsilon \hat{B}_{00}(k) + o_{00}(\varepsilon) & \varepsilon \hat{B}_{01}(k) + o_{01}(\varepsilon) \\ \varepsilon \hat{B}_{10}(k) + o_{10}(\varepsilon) & B_{11} + \varepsilon \hat{B}_{11}(k) + o_{11}(\varepsilon) \end{bmatrix}, \quad \varepsilon > 0, \quad \operatorname{Im} k > 0, \tag{1.3.15}$$

where the decomposition is with respect to $\mathscr{H}_0$ and $(\mathscr{H}_1 \dot{+} \mathscr{H}_2)$. Now let

$$\hat{B}_\varepsilon(k) = \begin{bmatrix} -1 + \hat{B}_{00}(k) + \dfrac{1}{\varepsilon} o_{00}(\varepsilon) & \varepsilon \hat{B}_{01}(k) + o_{01}(\varepsilon) \\ \hat{B}_{10}(k) + \dfrac{1}{\varepsilon} o_{10}(\varepsilon) & B_{11}(k) + \varepsilon \hat{B}_{11}(k) + o_{11}(\varepsilon) \end{bmatrix},$$

$$\varepsilon > 0, \quad \operatorname{Im} k > 0. \tag{1.3.16}$$

With these definitions we infer

$$[1 + B_\varepsilon(k)] \begin{bmatrix} \psi_0 \\ \varepsilon \psi_2 \end{bmatrix} = \varepsilon [1 + \hat{B}_\varepsilon(k)] \begin{bmatrix} \psi_0 \\ \psi_1 \end{bmatrix}. \tag{1.3.17}$$

By relabeling, if necessary, we can assume that $H_j = -\Delta \dot{+} V_j, j = 1, \ldots, n_0, n_0 \leq N$, are all in case II or IV. In addition, we also write ϕ_j for ϕ_{j1} if H_j is in case IV. With all this at hand, a typical element Ψ_0 and $\mathscr{H}_0$ looks like

$$\Psi_0 = \left(\frac{a_1}{(v_1, \phi_1)} \phi_1, \ldots, \frac{a_{n_0}}{(v_{n_0}, \phi_{n_0})} \phi_{n_0} \right) \tag{1.3.18}$$

and hence

$$(\hat{B}_{00}(k)\Psi_0)_j = (\phi_j, v_j)\phi_j \sum_{j'=1}^{n_0} \left[\left(\alpha_j - \frac{ik}{4\pi} \right) \delta_{jj'} - \tilde{G}_k(y_j - y_{j'}) \right] a_{j'}. \tag{1.3.19}$$

Furthermore, we observe that

$$\hat{B}_{10}(k)\Psi_0 + (1 + B_{11})\Psi_1 = 0 \tag{1.3.20}$$

can always be solved with respect to $\Psi_1 \in \mathscr{H}_1 \dot{+} \mathscr{H}_2$ for any $\Psi_0 \in \mathscr{H}_0$ since $\hat{B}_{10}(k)\Psi_0 \in \mathscr{H}_2$ and $[1 + B]|_{\mathscr{H}_2}$ is bijective from (1.3.12).

Hence

$$-1 \in \sigma(\hat{B}_0(k)) \quad \text{iff} \quad \operatorname{Ker} \hat{B}_{00}(k) \neq \{0\}. \tag{1.3.21}$$

What we have obtained so far is to replace the operator $B_\varepsilon(k)$, which contains no information on k when $\varepsilon = 0$, by the operator $\hat{B}_\varepsilon(k)$ which is directly related to the point interaction Hamiltonian $-\Delta_{\alpha,Y}$ at $\varepsilon = 0$. Let

$$d(\varepsilon, k) = \det_2[1 + \hat{B}_\varepsilon(k)], \tag{1.3.22}$$

which is analytic in ε and k near $\varepsilon = 0$ and in $\operatorname{Im} k > 0$. Then

$$\begin{aligned} d(0, k) &= \det_2\begin{bmatrix} 1 + [\hat{B}_{00}(k) - 1] & 0 \\ \hat{B}_{10}(k) & 1 + B_{11} \end{bmatrix} \\ &= \det_2\begin{bmatrix} 1 + [\hat{B}_{00}(k) - 1] & 0 \\ \hat{B}_{10}(k) & 1 \end{bmatrix} \det_2\begin{bmatrix} 1 & 0 \\ 0 & 1 + B_{11} \end{bmatrix} \\ &= \det_2[\hat{B}_{00}(k)] \det_2[1 + B_{11}] \\ &= \det[\hat{B}_{00}(k)] e^{-\operatorname{Tr}[\hat{B}_{00}(k) - 1]} \det_2(1 + B_{11}) \end{aligned} \tag{1.3.23}$$

using the relations ($\mathscr{H}$ being a separable Hilbert space)

$$\det_2\{[1 + A][1 + B]\} = \det_2[1 + A] \det_2[1 + B] \exp(-\operatorname{Tr} AB), \qquad A, B \in \mathscr{B}_2(\mathscr{H}), \tag{1.3.24}$$

$$\det_2[1 + A] = \det[1 + A] e^{-\operatorname{Tr} A}, \qquad A \in \mathscr{B}_1(\mathscr{H}). \tag{1.3.25}$$

None of the terms on the right-hand side of (1.3.23) can be zero except the first, and we can conclude that the multiplicity of the eigenvalue k_0^2 of $-\Delta_{\alpha,Y}$ equals the multiplicity of the zero of $d(0, k)$ at $k = k_0$.

Using the implicit function theorem we obtain that $H_{\varepsilon,Y}$ has exactly M eigenvalues (counting multiplicities) $k_{j,\varepsilon}^2$ converging to k_0^2, and that $k_{j,\varepsilon}^2$ can be expanded in a convergent Puiseux series. From Lemma B.4(a) we infer that this Puiseux series can have at most square root branch points and hence we obtain the expansion (1.3.1). To find the first coefficient in expansion (1.3.1) we proceed as follows. Let

$$\tilde{k}_{l,\varepsilon} = k_{l,\varepsilon^{m_l}}. \tag{1.3.26}$$

Then $\tilde{k}_{l,\varepsilon}$ and hence $B_{\varepsilon^m}(\tilde{k}_\varepsilon)$ (we suppress the l dependence in the notation) are analytic in ε near $\varepsilon = 0$. By first reducing the problem to a finite dimensional space by standard means ([391], Sects. XII.1 and XII.2) and using a theorem by Baumgärtel [60], [61] we can find an eigenvector Φ_ε near $\varepsilon = 0$ for $B_{\varepsilon^m}(\tilde{k}_\varepsilon)$ such that $\varepsilon \to \Phi_\varepsilon$ is analytic and

$$[1 + B_{\varepsilon^m}(\tilde{k}_\varepsilon)]\Phi_\varepsilon = 0. \tag{1.3.27}$$

Let $\Phi_\varepsilon = (\phi_{1,\varepsilon}, \ldots, \phi_{N,\varepsilon})$. Using (1.3.17) we can choose $\phi_{j,0} = 0, j = n_0 + 1, \ldots, N$, and

$$\phi_{j,0} = (v_j, \phi_j)^{-1} c_j \phi_j, \qquad j = 1, \ldots, n_0, \tag{1.3.28}$$

where $\phi_j, j = 1, \ldots, n_0$, are defined as in (1.3.18) and $(c_1, \ldots, c_{n_0})$ is an eigenvector of the matrix $\Gamma_{\alpha,Y}(k_0)$, i.e.,

$$\sum_{j'=1}^{n_0} \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_{k_0}(y_j - y_{j'})\right] c_{j'} = 0, \qquad j = 1, \ldots, n_0. \tag{1.3.29}$$

(Recall that, by assumption, H_j belong to case I or III for $j = n_0 + 1, \ldots, N$, and therefore do not contribute to the limit, or equivalently, $\alpha_j = \infty$ for $j = n_0 + 1, \ldots, N$.) Because of the resonances (Theorems 1.3.3 and 1.3.4) we will not use that $m \in \{1, 2\}$, but consider the general case $m \in \mathbb{N}$. By first taking the derivative m times with respect to ε at $\varepsilon = 0$ we obtain after a short computation denoting

$$k_1 = \frac{d\tilde{k}_\varepsilon}{d\varepsilon}\bigg|_{\varepsilon=0},$$

$$\phi_j^{(r)} = \frac{\partial^r \phi_{j,\varepsilon}}{\partial \varepsilon^r}\bigg|_{\varepsilon=0}, \qquad r = 2, \ldots, m+1, \quad j = 1, \ldots, N, \tag{1.3.30}$$

$$\phi_j' = \frac{\partial \phi_{j,\varepsilon}}{\partial \varepsilon}\bigg|_{\varepsilon=0}, \qquad j = 1, \ldots, N,$$

that

$$(1 + u_j G_0 v_j)\phi_j^{(m)} + m!\left[-\lambda_j'(0)(v_j, \phi_j)^{-1}\phi_j + \frac{ik_0}{4\pi}u_j\right]c_j$$
$$+ m! \sum_{j'=1}^{n_0} u_j \tilde{G}_{k_0}(y_j - y_{j'})c_{j'} = 0, \qquad j = 1, \ldots, n_0. \tag{1.3.31}$$

$m = 1$:

By taking the inner product with $\tilde{\phi}_j = \phi_j \operatorname{sgn} V_j$ we obtain of course (1.3.29). From (1.3.31) we deduce that

$$\phi_j' = \sum_{l=1}^{N_j} a_{jl}\phi_{jl} - \frac{1}{m!}T_j\left\{\left[-\lambda_j'(0)(u_j, \phi_j)^{-1}\phi_j + \frac{ik_0}{4\pi}u_j\right]c_j + \sum_{j'=1}^{n_0} u_j \tilde{G}_{k_0}(y_j - y_{j'})c_{j'}\right\}$$
$$\equiv a_j\phi_j + \sum_{l=2}^{N_j} a_{jl}\phi_{jl} + \chi_j, \qquad j = 1, \ldots, n_0, \tag{1.3.32}$$

where T_j denotes the reduced resolvent (cf. (I.1.2.37)) with V replaced by $V_j, j = 1, \ldots, n_0$, and where $a_1, \ldots, a_{n_0}$ are constants to be determined later and a_{jl}, $l = 2, \ldots, N_j$, $j = 1, \ldots, n_0$, are constants which will drop out of the subsequent calculations. By calculating the second derivative of (1.3.27) in $\varepsilon = 0$ and taking the inner product with $\tilde{\phi}_j$ we finally obtain

$$\lambda_j''(0)(v_j, \phi_j)^{-1}c_j - \frac{k_0^2}{4\pi}\int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_j(x)}v_j(x)|x - x'|v_j(x')\phi_j(x')(v_j, \phi_j)^{-1}c_j$$
$$+ (\phi_j, v_j)\lambda_j'(0)\alpha_j c_j + \lambda_j'(0)a_j - \lambda_j'(0)(\tilde{\phi}_j, \chi_j)$$
$$+ 2\sum_{j'=1}^{n_0} \tilde{G}_{k_0}(y_j - y_{j'})(\phi_j, v_j)[(v_{j'}, \phi_{j'})a_{j'} + (v_{j'}, \chi_{j'})]$$
$$+ \frac{ik_0}{4\pi}|(\phi_j, v_j)|^2 a_j - \frac{ik_0}{4\pi}(\phi_j, v_j)(v_j, \chi_j) + \frac{ik_1}{4\pi}(\phi_j, v_j)\sum_{j'=1}^{n_0} e^{ik_0|y_j - y_{j'}|}c_{j'}$$
$$+ \sum_{j'=1}^{n_0}\int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi_j(x)}v_j(x)\nabla\tilde{G}_{k_0}(y_j - y_{j'})\cdot$$
$$\cdot(x - x')v_{j'}(x')\phi_{j'}(x')(v_{j'}, \phi_{j'})^{-1}c_{j'} = 0, \qquad j = 1, \ldots, n_0. \tag{1.3.33}$$

This is a system of n_0 equations with $n_0 + 1$ unknowns (k_1 and $a_1, \ldots, a_{n_0}$). However, there is still one overall constant left undetermined, namely the normalization of Φ_ε (or the eigenvector $(c_1, \ldots, c_n)$). This reduces the number of unknowns to n_0.

$m > 1$:

First, we observe that

$$(1 + u_j G_0 v_j)\phi_j' = 0 \tag{1.3.34}$$

and hence

$$\phi_j' = a_j\phi_j + \sum_{l=2}^{N_j} a_{jl}\phi_{jl}, \qquad j = 1, \ldots, n_0 \tag{1.3.35}$$

for some constants $(a_1, \ldots, a_{n_0})$ to be determined later (the constants a_{jl}, $l = 2, \ldots, N_j$, $j = 1, \ldots, n_0$, will cancel). By computing the $(m + 1)$th derivative of (1.3.27) in $\varepsilon = 0$ we obtain, after taking the inner product with $\tilde{\phi}_j$, that

$$\frac{ik_0}{4\pi}|(\phi_j, v_j)|^2 a_j + \lambda_j'(0)a_j + (\phi_j, v_j)\sum_{j'=1}^{n_0} \tilde{G}_{k_0}(y_j - y_{j'})(v_{j'}, \phi_{j'})a_{j'}$$

$$+ \frac{ik_1}{4\pi}(\phi_j, v_j)\sum_{j'=1}^{n_0} e^{ik_0|y_j - y_{j'}|}c_{j'} = 0, \qquad j = 1, \ldots, n_0. \tag{1.3.36}$$

Again this is a system of n_0 equations with $n_0 + 1$ unknowns $(k_1, a_1, \ldots, a_{n_0})$ which is still solvable due to the one extra degree of freedom contained in the normalization of Φ_ε. ∎

Turning the situation the other way around we can start with the negative eigenvalues of $H_{\varepsilon,Y}$ which remain bounded and do not get absorbed in the continuous part of the spectrum as $\varepsilon \downarrow 0$. This is the set-up for the next theorem.

Theorem 1.3.2. *Let $V_j \in R$ be real-valued,* supp V_j *compact, $j = 1, \ldots, N$, and suppose* (I.1.2.84). *Moreover, if $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV *for some j we assume, in addition, $\lambda_j'(0) \neq 0$. Let E_ε be a negative eigenvalue of $H_{\varepsilon,Y}$ such that*

$$-\infty < M_1 \leq E_\varepsilon \leq M_2 < 0 \tag{1.3.37}$$

for $\varepsilon > 0$ small enough. Suppose $\{\varepsilon_n\}$ is a positive sequence decreasing to zero, and denote by k_0^2 ($\operatorname{Im} k_0 > 0$*) any accumulation point for $\{E_{\varepsilon_n}\}$. Then k_0^2 is an eigenvalue of $-\Delta_{\alpha,Y}$. Let M be the multiplicity of the eigenvalue k_0^2 of $-\Delta_{\alpha,Y}$. Then the conclusion of Theorem* 1.3.1 *holds, i.e., there exist m analytic functions h_l, $l = 1, \ldots, m$, with $h_l(0) = 0$ such that for $m_l \in \{1, 2\}$, $l = 1, \ldots, m$,*

$$\begin{aligned} k_{l,\varepsilon}^2 &= k_0^2 + h_l(\varepsilon^{1/m_l}) \\ &= k_0^2 + \sum_{r=1}^{\infty} a_{l,r}\varepsilon^{r/m_l}, \qquad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M, \end{aligned} \tag{1.3.38}$$

are all the eigenvalues of $H_{\varepsilon,Y}$ near k_0^2. $k_{l,\varepsilon}$ can expanded as in (1.3.2). *In particular, $2^{-1}a_{l,1} = k_1$ is given by* (1.3.33) *if $m_l = 1$ and by* (1.3.36) *if $m_l > 1$.*

PROOF. The proof is almost a direct consequence of the proof of Theorem 1.3.1. In the notation of that proof the analytic function

$$d(\varepsilon, k) = \det_2[1 + \hat{B}_\varepsilon(k)] \tag{1.3.39}$$

is zero iff k^2 is an eigenvalue of $H_{\varepsilon,Y}$ when $\varepsilon > 0$, and of $-\Delta_{\alpha,Y}$ if $\varepsilon = 0$. From the assumptions we know that

$$\varepsilon_n \downarrow 0, \qquad d(\varepsilon_n, \sqrt{E_{\varepsilon_n}}) = 0, \qquad \operatorname{Im} \sqrt{E_{\varepsilon_n}} > 0, \tag{1.3.40}$$

and that $E_{\varepsilon_n} \to k_0^2$. Hence

$$d(0, k_0) = 0, \qquad \operatorname{Im} k_0 > 0, \tag{1.3.41}$$

and we are in the situation covered by Theorem 1.3.1 for obtaining the stated form of $k_{l,\varepsilon}$. ∎

In the proofs of Theorems 1.3.1. and 1.3.2 we did not use in an essential way that k_ε^2 was an eigenvalue of $H_{\varepsilon,Y}$ *per se*, but only the equivalent statement that $B_\varepsilon(k_\varepsilon)$ had -1 as an eigenvalue. But in the "unphysical half-plane" (i.e., in $\operatorname{Im} k < 0$) this is by definition equivalent to k_ε being a resonance of $H_{\varepsilon,Y}$. Thus we can immediately state the analogous results of Theorems 1.3.1 and 1.3.2 for resonances.

Theorem 1.3.3. *Let $V_j \in R$ be real-valued,* supp V_j *compact, $j = 1, \ldots, N$, and suppose* (I.1.2.84). *Moreover, if $H_j = -\Delta \dotplus V_j$ is in case* III *of* IV *for some j we assume, in addition, $\lambda_j'(0) \neq 0$. Let k_0,* $\operatorname{Im} k_0 < 0$, *be a resonance of $-\Delta_{\alpha,Y}$ of multiplicity M. Then $H_{\varepsilon,Y}$ has exactly M resonances which are branches of one or more multivalued analytic functions with at most an algebraic branch point at $\varepsilon = 0$,* such that

$$\begin{aligned} k_{l,\varepsilon} &= k_0 + h_l(\varepsilon^{1/m_l}) \\ &= k_0 + \sum_{r=1}^{\infty} a_{l,r}\varepsilon^{r/m_l}, \qquad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M, \end{aligned} \tag{1.3.42}$$

are all the resonances of $H_{\varepsilon,Y}$ near k_0 for $\varepsilon > 0$ sufficiently small. Furthermore, $a_{l,1} = k_1$ is given as a solution of (1.3.33) *if $m_l = 1$ and of* (1.3.36) *if $m_l > 1$.*

Remark. We cannot infer that $m_l \in \{1, 2\}$ in this case as we could for the eigenvalues, because we no longer have the constraint that $k_\varepsilon \in i\mathbb{R}$ for $\varepsilon > 0$ small enough.

Proof. As in the proof of Theorem 1.3.1 we define

$$d(\varepsilon, k) = \det{}_2[1 + \hat{B}_\varepsilon(k)], \tag{1.3.43}$$

and from the assumption we have

$$d(0, k_0) = 0, \qquad d(0, \cdot) \not\equiv 0 \tag{1.3.44}$$

which, using the implicit function theorem, implies (1.3.42). The expansion is obtained as in Theorem 1.3.1. ∎

Theorem 1.3.4. *Let $V_j \in R$ be real-valued,* supp V_j *compact, $j = 1, \ldots, N$, and suppose* (I.1.2.84). *Moreover, if $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV *for some j we assume, in addition, $\lambda_j'(0) \neq 0$. Let k_ε,* $\operatorname{Im} k_\varepsilon < 0$, *be a resonance of $H_{\varepsilon,Y}$ such that*

$$0 < M_1 \leq |\operatorname{Im} k_\varepsilon| \leq |k_\varepsilon| \leq M_2 < \infty \tag{1.3.45}$$

for ε small enough. Suppose $\{\varepsilon_n\}$ is a positive sequence decreasing to zero. Then any accumulation point k_0 of $\{k_{\varepsilon_n}\}$ is a resonance of $-\Delta_{\alpha,Y}$. Let M denote the multiplicity of k_0. Then there exist m analytic functions h_l, $l = 1, \ldots, m$, with $h_l(0) = 0$ such that

$$k_{l,\varepsilon} = k_0 + h_l(\varepsilon^{1/m_l})$$

$$= k_0 + \sum_{r=1}^{\infty} a_{l,r}\varepsilon^{r/m_l}, \qquad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M, \tag{1.3.46}$$

are all the resonances of $H_{\varepsilon,Y}$ near k_0. $a_{l,1} = k_1$ is given by (1.3.33) *if $m_l = 1$ and by* (1.3.36) *if $m_l > 1$.*

Proof. The proof is essentially equal to that of Theorem 1.3.2. ■

II.1.4 Multiple Well Problems

By the multiple well problem we mean the asymptotic study of eigenvalues and resonances of the operator

$$H_Y(\varepsilon) = -\Delta \dotplus \sum_{j=1}^{N} V_j(\cdot - \varepsilon^{-1}y_j), \qquad \varepsilon > 0, \tag{1.4.1}$$

as $\varepsilon \downarrow 0$. Assuming that the potentials V_j are localized around the origin, the operator $H_Y(\varepsilon)$ corresponds to the situation where the centers $y_1/\varepsilon, \ldots, y_N/\varepsilon$, around which the potentials $V_1(\cdot - \varepsilon^{-1}y_1), \ldots, V_N(\cdot - \varepsilon^{-1}y_N)$ are concentrated, move apart.

The reason why we can study this problem in the context of point interactions is, of course, the scaling relation we have noted and employed earlier, viz., if

$$H_{\varepsilon,Y} = -\Delta \dotplus \varepsilon^{-2} \sum_{j=1}^{N} V_j(\varepsilon^{-1}(\cdot - y_j)), \qquad \varepsilon > 0, \tag{1.4.2}$$

then

$$H_Y(\varepsilon) = \varepsilon^2 U_\varepsilon^{-1} H_{\varepsilon,Y} U_\varepsilon, \tag{1.4.3}$$

where U_ε is the unitary scaling group given by (1.2.3). We will begin with what we would like to call the *critical multiple well problem*, i.e., where we, in addition, assume that

$$H_j = -\Delta \dotplus V_j, \qquad j = 1, \ldots, N, \tag{1.4.4}$$

is in case II, i.e., H_j has a simple zero-energy resonance. In the preceding section we treated the case when

$$k_\varepsilon^2 \to k_0^2 < 0 \quad \text{as } \varepsilon \downarrow 0, \tag{1.4.5}$$

where k_ε^2 is an eigenvalue of $H_{\varepsilon,Y}$. From the unitary equivalence (1.4.3) we infer that if $k^2(\varepsilon)$ ($\operatorname{Im} k(\varepsilon) > 0$) denotes an eigenvalue of $H_Y(\varepsilon)$, we have the relation

$$k_\varepsilon = \varepsilon^{-1}k(\varepsilon) \tag{1.4.6}$$

which implies that we have studied eigenvalues of $H_Y(\varepsilon)$ approaching zero as $O(\varepsilon^2)$. For the critical double well ($N = 2$, $y_1 = 0$, $y_2 = y$, in (1.4.1)) we can immediately state the following theorem.

Theorem 1.4.1. *Let*

$$H_y(\varepsilon) = -\Delta \dotplus V_1 \dotplus V_2(\cdot - \varepsilon^{-1}y), \tag{1.4.7}$$

where $V_j \in R$, $j = 1, 2$, are real-valued and of compact support. Moreover, assume that $H_j = -\Delta \dotplus V_j$, $j = 1, 2$, are in case II. *Then $H_y(\varepsilon)$ has, for $\varepsilon > 0$ sufficiently small, a simple eigenvalue $k^2(\varepsilon)$,* Im $k(\varepsilon) > 0$, *tending to zero as*

$$k(\varepsilon) = \varepsilon k_0 + \varepsilon^2 k_1 + o(\varepsilon^2), \tag{1.4.8}$$

where k_0 is the unique solution with Im $k_0 > 0$ *of*

$$ik_0 |y| = -e^{ik_0|y|}. \tag{1.4.9}$$

In addition, $H_y(\varepsilon)$ has an infinite sequence of simple resonances $k_n(\varepsilon)$ tending to zero and

$$k_n(\varepsilon) = \varepsilon k_{0,n} + \varepsilon^2 k_{1,n} + o(\varepsilon^2), \tag{1.4.10}$$

where $k_{0,n}$ is a solution with Im $k_{0,n} < 0$ *of*

$$ik_{0,n}|y| = \pm e^{ik_{0,n}|y|}. \tag{1.4.11}$$

k_1 and $k_{1,n}$ are solutions of (1.3.33). *Asymptotically, we have*

$$k_{0,n} \approx \frac{1}{|y|}(n + \tfrac{1}{2})\pi - \frac{i}{|y|} \ln[(n + \tfrac{1}{2})\pi] \quad \text{as } n \to \infty. \tag{1.4.12}$$

Remark. The numerical values of the solutions of

$$iz_n = \pm e^{iz_n} \tag{1.4.13}$$

with Re $z_n \geq 0$, for the first few n, are given in Table 1.

PROOF. Since now, according to our notation, $\lambda_j(\varepsilon) \equiv 1$, which implies that $\alpha_1 = \alpha_2 = 0$, we combine the computations from the example in Sect. 1.1 with Theorems 1.3.1 and 1.3.2 to obtain the result. ■

For completeness we state a similar result in the N-center case.

Theorem 1.4.2. *Let*

$$H_Y(\varepsilon) = -\Delta \dotplus \sum_{j=1}^{N} V_j(\cdot - \varepsilon^{-1}y_j), \qquad \varepsilon > 0,$$

where $V_j \in R$ are real-valued and have compact support for $j = 1, \ldots, N$. In addition assume that $H_j = -\Delta \dotplus V_j$ is in case II *for $j = 1, \ldots, N$. Then we have:*

(a) *If $H_Y(\varepsilon)$ has a continuous eigenvalue $k^2(\varepsilon)$ (resp. resonance $k(\varepsilon)$) such that*

$$0 < M_1 \leq |\text{Im } k(\varepsilon)| \varepsilon^{-1} \leq |k(\varepsilon)| \varepsilon^{-1} \leq M_2 < \infty \tag{1.4.14}$$

for ε small enough, then $k(\varepsilon)$ is a multivalued analytic function and we have the expansion

$$k(\varepsilon) = \varepsilon k_0 + \varepsilon^{(m+1)/m} k_1 + o(\varepsilon^{(m+1)/m}), \tag{1.4.15}$$

where k_0, $\operatorname{Im} k_0 > 0$ (resp. $\operatorname{Im} k_0 < 0$), is a solution of

$$\det\left[\frac{ik_0}{4\pi}\delta_{jj'} + \tilde{G}_{k_0}(y_j - y_{j'})\right] = 0 \tag{1.4.16}$$

and k_1 is a solution of (1.3.33) *if $m = 1$ and of* (1.3.36) *if $m > 1$. (If $\operatorname{Im} k_0 > 0$, then $1 \le m \le 2$.)*

(b) *If k_0 is a solution of* (1.4.16), *then there exists an eigenvalue $k^2(\varepsilon)$ of $H_Y(\varepsilon)$ if $\operatorname{Im} k_0 > 0$ (resp. a resonance $k(\varepsilon)$ if $\operatorname{Im} k_0 < 0$) with the expansion* (1.4.15).

PROOF. The theorem is a direct consequence of Theorems 1.3.1–1.3.4 by noting that (1.4.16) is equivalent to the statement that k_0^2 is an eigenvalue (resp. k_0 is a resonance) of $-\Delta_{0,Y}$. ∎

Table 1

n	$\frac{1}{\pi}\operatorname{Re} z_n$	$\operatorname{Im} z_n$
0	0	0.567143
1	0.425655	−0.318132
2	1.392665	−1.533913
3	2.415536	−2.062278
4	3.430203	−2.401585
5	4.440171	−2.653192
6	5.447408	−2.853582
7	6.452924	−3.020240
8	7.457284	−3.162953
9	8.460827	−3.287769
10	9.463770	−3.398692
11	10.466259	−3.498515
12	11.468394	−3.589263
13	12.470248	−3.672450
14	13.471876	−3.749243
15	14.473317	−3.820554
16	15.474603	−3.887116
17	16.475759	−3.949523
18	17.476803	−4.008262
19	18.477753	−4.063742
20	19.488621	−4.116305
21	20.479416	−4.166242

II.1.5 Stationary Scattering Theory

The topic of this section is the study of scattering quantities for the Schrödinger operator with point interactions at a finite number of points in $\mathbb{R}^3$ and their natural ε-expansions. We start with stationary scattering theory for the pair

$(-\Delta_{\alpha,Y}, -\Delta)$. Let

$$\Psi_{\alpha,Y}(k\omega, x) = e^{ik\omega x} + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} e^{ik\omega y_{j'}} \frac{e^{ik|x-y_j|}}{4\pi|x-y_j|},$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k \geq 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad x \notin Y, \quad \omega \in S^2. \tag{1.5.1}$$

Then $\Psi_{\alpha,Y}$ is formally of the form (1.1.43) with $\phi_k(x) = e^{ik\omega x}$ which is not in $L^2(\mathbb{R}^3)$ but satisfies

$$(-\Delta\phi_k)(x) = k^2\phi_k(x) \tag{1.5.2}$$

in the distributional sense. Furthermore,

$$(-\Delta\Psi_{\alpha,Y})(k\omega, x) = k^2\Psi_{\alpha,Y}(k\omega, x), \qquad x \notin Y, \tag{1.5.3}$$

and

$$\lim_{\varepsilon\downarrow 0} \lim_{\substack{|x'|\to\infty \\ -|x'|^{-1}x'=\omega}} 4\pi|x'|e^{-i(k+i\varepsilon)|x'|}[-\Delta_{\alpha,Y} - (k+i\varepsilon)^2]^{-1}(x, x') = \Psi_{\alpha,Y}(k\omega, x),$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k \geq 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad x \notin Y. \tag{1.5.4}$$

Hence the functions $\Psi_{\alpha,Y}$ constitute the generalized eigenfunctions of $-\Delta_{\alpha,Y}$ or, in other words, the scattering wave functions. With this at hand the *on-shell scattering amplitude* $f_{\alpha,Y}(k, \omega, \omega')$ associated with $-\Delta_{\alpha,Y}$ equals

$$\begin{aligned} f_{\alpha,Y}(k, \omega, \omega') &= \lim_{\substack{|x|\to\infty \\ |x|^{-1}x=\omega}} |x|e^{-ik|x|}[\Psi_{\alpha,Y}(k\omega', x) - e^{ik\omega' x}] \\ &= (4\pi)^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} e^{ik(y_{j'}\omega' - y_j\omega)}, \end{aligned}$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k \geq 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad \omega, \omega' \in S^2. \tag{1.5.5}$$

Hence the *off-shell extension* $f_{\alpha,Y}(k, p, q)$ of $f_{\alpha,Y}(k, \omega, \omega')$ reads

$$f_{\alpha,Y}(k, p, q) = (4\pi)^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} e^{i(y_{j'}q - y_j p)},$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k \in \mathbb{C}, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad p, q \in \mathbb{C}^3, \tag{1.5.6}$$

so as to make

$$f_{\alpha,Y}(k, \omega, \omega') = f_{\alpha,Y}(k, p, q)|_{|p|=|q|=k},$$

$$p, q \in \mathbb{R}^3, \quad \omega = |p|^{-1}p, \quad \omega' = |q|^{-1}q. \tag{1.5.7}$$

Thus the unitary *on-shell scattering operator* $\mathscr{S}_{\alpha,Y}(k)$ in $L^2(S^2)$ equals

$$(\mathscr{S}_{\alpha,Y}(k)\phi)(\omega) = \phi(\omega) - \frac{k}{2\pi i}\int_{S^2} d^2\omega' f_{\alpha,Y}(k, \omega, \omega')\phi(\omega'), \qquad \phi \in L^2(S^2), \tag{1.5.8}$$

or after insertion of (1.5.5)

$$\mathscr{S}_{\alpha,Y}(k) = 1 - (k/8\pi^2 i) \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(e^{-iky_{j'}(\cdot)}, \cdot)e^{-iky_j(\cdot)}$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k \geq 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N. \quad (1.5.9)$$

The low-energy limits of $f_{\alpha,Y}(k, \omega, \omega')$ and $\mathscr{S}_{\alpha,Y}(k)$ can easily be obtained from (1.5.5) and (1.5.9), respectively. Namely, we have

$$\operatorname*{n-lim}_{k\to 0} \mathscr{S}_{\alpha,Y}(k) = 1,$$

$$-\lim_{k\to 0} f_{\alpha,Y}(k, \omega, \omega') = -(4\pi)^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(0)]_{jj'}^{-1} = a_{\alpha,Y},$$

$$\det[\Gamma_{\alpha,Y}(0)] \neq 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad (1.5.10)$$

where $a_{\alpha,Y}$ is the scattering length. Finally, we observe that $\mathscr{S}_{\alpha,Y}$ has a meromorphic continuation in k to $\mathbb{C}$ with poles exactly at the eigenvalues and resonances of $-\Delta_{\alpha,Y}$.

We now turn to the question of how the scattering amplitude $f_{\alpha,Y}$ and the on-shell scattering operator $\mathscr{S}_{\alpha,Y}$ are approximated by the corresponding quantities for the operator $H_{\varepsilon,Y}$. First, let

$$\tilde{\Phi}_{0,\varepsilon}^{\pm}(p, x) = (\tilde{\phi}_{\varepsilon,y_1}^{\pm}(p, x), \ldots, \tilde{\phi}_{\varepsilon,y_N}^{\pm}(p, x)), \quad (1.5.11)$$

where

$$\tilde{\phi}_{\varepsilon,y_j}^{+}(p, x) = \tilde{u}_{\varepsilon,j}(x)e^{ipx}, \qquad \tilde{\phi}_{\varepsilon,y_j}^{-}(p, x) = \tilde{v}_{\varepsilon,j}(x)e^{ipx},$$

$$\tilde{u}_{\varepsilon,j}(x) = \tilde{u}_j((x - y_j)/\varepsilon), \qquad \tilde{v}_{\varepsilon,j}(x) = \tilde{v}_j((x - y_j)/\varepsilon);$$

$$\varepsilon > 0, \quad x \in \mathbb{R}^3, \quad p \in \mathbb{C}^3, \quad j = 1, \ldots, N, \quad (1.5.12)$$

and $\tilde{u}_j$ and $\tilde{v}_j$ are defined by (1.2.11) and $V_j \in R$ are real-valued with supp V_j compact, $j = 1, \ldots, N$. The transition operator $\tilde{t}_{\varepsilon,Y}(k)$ for $H_{\varepsilon,Y}$ then reads

$$\tilde{t}_{\varepsilon,Y}(k) = [\tilde{t}_{\varepsilon,jj'}(k)]_{j,j'=1}^{N}: \mathscr{H} \to \mathscr{H}, \qquad \tilde{t}_{\varepsilon,jj'}(k) = \varepsilon^{-2}\lambda_j(\varepsilon)[1 + B(\varepsilon, k)]_{jj'}^{-1}$$

$$\varepsilon > 0, \quad \operatorname{Im} k \geq 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad j, j' = 1, \ldots, N, \quad (1.5.13)$$

where

$$B(\varepsilon, k) = [B_{jj'}(\varepsilon, k)]_{j,j'=1}^{N}: \mathscr{H} \to \mathscr{H},$$
$$B_{jj'}(\varepsilon, k) = \varepsilon^{-2}\lambda_j(\varepsilon)\tilde{u}_{\varepsilon,j}G_k\tilde{v}_{\varepsilon,j'}, \qquad \varepsilon > 0, \quad \operatorname{Im} k \geq 0, \quad j, j' = 1, \ldots, N, \quad (1.5.14)$$

and

$$\mathscr{E}_\varepsilon = \{k^2 \in \mathbb{C} - \{0\} \mid -1 \in \sigma_p(B(\varepsilon, k)), \operatorname{Im} k \geq 0\} \quad (1.5.15)$$

which is a discrete, compact set of zero Lebesgue measure.

Then the on-shell scattering amplitude $f_{\varepsilon,Y}(k, \omega, \omega')$ of $H_{\varepsilon,Y}$ reads

$$f_{\varepsilon,Y}(k, \omega, \omega') = -(4\pi)^{-1}(\tilde{\Phi}_{0,\varepsilon}^{-}(k\omega), \tilde{t}_{\varepsilon,Y}(k)\tilde{\Phi}_{0,\varepsilon}^{+}(k\omega'))$$

$$= -(4\pi)^{-1} \sum_{j,j'=1}^{N} (\tilde{\phi}_{\varepsilon,y_j}^{-}(k\omega), \tilde{t}_{\varepsilon,jj'}(k)\tilde{\phi}_{\varepsilon,y_{j'}}^{+}) \quad (1.5.16)$$

with its off-shell extension $f_{\varepsilon,Y}(k, p, q)$ given by

$$f_{\varepsilon,Y}(k, p, q) = -(4\pi)^{-1}(\tilde{\Phi}_{0,\varepsilon}^{-}(p), \tilde{t}_{\varepsilon,Y}(k)\tilde{\Phi}_{0,\varepsilon}^{+}(q))$$
$$= -(4\pi)^{-1} \sum_{j,j'=1}^{N} (\tilde{\phi}_{\varepsilon,y_j}^{-}(p), \tilde{t}_{\varepsilon,jj'}(k)\tilde{\phi}_{\varepsilon,y_{j'}}^{+}(q)) \tag{1.5.17}$$

such that

$$f_{\varepsilon,Y}(k, \omega, \omega') = f_{\varepsilon,Y}(k, q, p)|_{|p|=|q|=k},$$
$$\varepsilon > 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad p, q \in \mathbb{R}^3, \quad \omega = |p|^{-1}p, \quad \omega' = |q|^{-1}q. \tag{1.5.18}$$

Finally, the unitary on-shell scattering operator $S_{\varepsilon,Y}(k)$ for $H_{\varepsilon,Y}$ equals

$$(S_{\varepsilon,Y}(k)\phi)(\omega) = \phi(\omega) - \frac{k}{2\pi i}\int_{S^2} d^2\omega'\, f_{\varepsilon,Y}(k, \omega, \omega')\phi(\omega'),$$
$$\phi \in L^2(S^2), \quad \varepsilon, k > 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad \omega \in S^2. \tag{1.5.19}$$

With all these definitions at hand we will start studying their relations in the $\varepsilon \downarrow 0$ limit. By performing the usual scaling, we transfer the difficult ε dependence from $\Phi_{0,\varepsilon}^{\pm}$ to the transition operator $t_{\varepsilon,Y}(k)$, so that the ε dependence essentially enters the explicit function $G_k(x)$.

Theorem 1.5.1. *Let $V_j \in R$ be real-valued with compact support for $j = 1, \ldots, N$ and suppose* (I.1.2.84). *If $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV *for some j, assume, in addition, that $\lambda_j'(0) \neq 0$. Then $f_{\varepsilon,Y}(k, p, q)$ is analytic in ε near $\varepsilon = 0$ and*

$$f_{\varepsilon,Y}(k, p, q) = f_{\alpha,Y}(k, p, q) + O(\varepsilon), \qquad \det[\Gamma_{\alpha,Y}(k)] \neq 0, \qquad k \geq 0, \quad p, q \in \mathbb{C}^3 \tag{1.5.20}$$

with α given by (1.2.6).

PROOF. Using the unitary scaling group U_ε defined by (1.2.3) and the unitary group of translations $T_{y_j/\varepsilon}$ defined by (1.2.13) we see that $f_{\varepsilon,Y}(k, p, q)$ can be written as

$$f_{\varepsilon,Y}(k, p, q)$$
$$= -(4\pi)^{-1} \sum_{j,j'=1}^{N} (U_\varepsilon^{-1}T_{y_j/\varepsilon}\tilde{\phi}_{\varepsilon,y_j}^{-}(p), U_\varepsilon^{-1}T_{y_j/\varepsilon}\tilde{t}_{\varepsilon,jj'}(k)T_{y_{j'}/\varepsilon}^{-1}U_\varepsilon U_\varepsilon^{-1}T_{y_{j'}/\varepsilon}\tilde{\phi}_{\varepsilon,y_j}^{+}(q))$$
$$= -(4\pi)^{-1} \sum_{j,j'=1}^{N} (\phi_{\varepsilon,y_j}^{-}(p), t_{\varepsilon,jj'}(k)\phi_{\varepsilon,y_{j'}}^{+}(q))$$
$$= -(4\pi)^{-1}\varepsilon(\Phi_{0,\varepsilon}^{-}(p), t_\varepsilon(k)\Phi_{0,\varepsilon}^{+}(q)). \tag{1.5.21}$$

Here

$$\Phi_{0,\varepsilon}^{\pm}(p) = (\phi_{\varepsilon,y_1}^{\pm}(p), \ldots, \phi_{\varepsilon,y_N}^{\pm}(p)), \tag{1.5.22}$$

and

$$\begin{aligned}
&\phi_{\varepsilon,y_j}^{+}(p, x) = u_j(x)e^{ip(\varepsilon x+y_j)}, \\
&\phi_{\varepsilon,y_j}^{-}(p, x) = v_j(x)e^{ip(\varepsilon x+y_j)}; \qquad \varepsilon > 0, \quad x \in \mathbb{R}^3, \quad p \in \mathbb{C}^3, \quad j = 1, \ldots, N,
\end{aligned} \tag{1.5.23}$$

and, finally,

$$t_\varepsilon(k) = [t_{\varepsilon,jj'}(k)]_{j,j'=1}^N : \mathscr{H} \to \mathscr{H}, \qquad t_{\varepsilon,jj'} = \lambda_j(\varepsilon)[1 + B_\varepsilon(k)]_{jj'}^{-1}, \tag{1.5.24}$$

where $B_\varepsilon(k)$ is defined in (1.2.9). Hence $f_{\varepsilon,Y}(k,p,q)$ is analytic in ε near $\varepsilon = 0$, and using (1.2.25) we obtain the limit (1.5.20). ∎

Remark. The next order in (1.5.20) can be computed explicitly (cf. [252]). We also emphasize our convention that the j_0th line and row should be deleted in the matrix $\Gamma_{\alpha,Y}(k)$ if $\alpha_{j_0} = \infty$ for some j_0.

Applying this theorem to the scattering operator, we immediately infer the following result.

Theorem 1.5.2. *Let $V_j \in R$ be real-valued with compact support for $j = 1, \ldots, N$ and suppose* (I.2.84). *If $H_j = -\Delta \dot{+} V_j$ is in case* III *or* IV *for some j, assume, in addition, that $\lambda_j'(0) \neq 0$. Then $S_{\varepsilon,Y}(k)$ is analytic in ε near $\varepsilon = 0$ and*

$$S_{\varepsilon,Y}(k) = \mathscr{S}_{\alpha,Y}(k) + O(\varepsilon), \qquad \det[\Gamma_{\alpha,Y}(k)] \neq 0, \qquad k \geq 0, \tag{1.5.25}$$

with α given by (1.2.6).

PROOF. Applying the definition (1.5.19) and Theorem 1.5.1 the result immediately follows. ∎

Notes

Section II.1.1

The N-center point interaction appears in the physics literature in [80], [132], [149], [151], [277], [363], [380]. In the mathematics literature the operator (1.1.33) was first studied by Albeverio, Fenstad, and Høegh-Krohn [12] using nonstandard analysis. Nonstandard analysis provides a justification of the heuristic computations made at the beginning of this chapter, see Appendix H. Our proof of Theorem 1.1.1 is essentially taken from Grossmann, Høegh-Krohn, and Mebkhout [226], see also [227]. Theorem 1.1.2 is due to Zorbas [512], see also [129], while Theorem 1.1.3 is contained in [227] and Theorem 1.1.4 is an extension of some of the corresponding results in [227] (cf. also [363]). Proposition 1.1.5 is taken from Thomas [482], [483], where one can also find more detailed estimates on $N(k^2, \alpha_1, \ldots, \alpha_N)$. The final example, the two-center problem, has been studied by [62], [146], [445], [463], [464], while our presentation closely follows Albeverio and Høegh-Krohn [26] where the regular three-center problem is also solved (cf. also [380]). Resonances in the N-center problem are also discussed in [432].

Apart from the proof in nonstandard analysis and the proof used here in order to define the Schrödinger operator with a finite number of point interactions, there are also other possibilities: One can simply start with the explicit expression (1.1.33) for the resolvent, and prove that this is the resolvent of a self-adjoint operator. This point of view has been used in Grossmann, Høegh-Krohn, and Mebkhout [227].

Another possibility is to use Theorem 1.1.2 as a starting point. This has been discussed by Zorbas [512] and, in particular, by [129]. In the latter, point interactions corresponding to other self-adjoint extensions are studied.

Finally, one can obtain the Schrödinger operator with point interactions as limits of Schrödinger operators with less singular short-range interactions. This is the content of Sect. II.1.2.

For generalized pointlike interactions, cf. [369], [370], and [430].

External electric fields in connection with $-\Delta_{\alpha, Y}$ are studied in [2].

Resonances in arrays as $N \to \infty$ are discussed in [228], [503].

Section II.1.2

The first result on the approximations of point interactions by local scaled short-range interactions in the N-center case was given by Albeverio and Høegh-Krohn [24]. Their result has been improved by Holden, Høegh-Krohn, and Johannesen [250] and the presentation here is a slight improvement on the latter.

Section II.1.3

The first results on the short-range expansion of eigenvalues and resonances in the N-center case appeared in Holden, Høegh-Krohn, and Johannesen [250]. The presentation here is an improvement on [250]. The location of resonances is also studied in [380].

Section II.1.4

The multiple well, and in particular the double well, has been studied for a long time in mathematical physics. Theorem 1.4.1 is due to Høegh-Krohn and Mebkhout [244], [245]. But the eigenvalue part was noted earlier by Klaus and Simon [297]. Klaus [295] obtained stronger results for the ground state of the symmetric double well, $H = -\Delta + V + V(\cdot - y)$. In [245] the asymptotic behavior of eigenvalues, resonances, and eigenvectors of the operator $H_y(\varepsilon)$ is studied.

Section II.1.5

The short-range expansion for the scattering amplitude and scattering operator was first discussed by Holden, Høegh-Krohn, and Mebkhout [252] where the next order terms are also explicitly computed. Furthermore, in the generic case, i.e., in case I, the third-order term is also calculated. Scattering from point interactions has been treated in [483].

CHAPTER II.2

Finitely Many δ-Interactions in One Dimension

II.2.1 Basic Properties

The purpose of this section is to generalize Sect. I.3.1 to the case of finitely many δ-interactions on the real line.

Let $N \in \mathbb{N}$ and introduce the set $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}$. The minimal operator $\dot{H}_Y$ in $L^2(\mathbb{R})$ is then defined by

$$\dot{H}_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}_Y) = \{g \in H^{2,2}(\mathbb{R}) | g(y_j) = 0, y_j \in Y, j = 1, \ldots, N\}. \tag{2.1.1}$$

$\dot{H}_Y$ is closed and nonnegative and its adjoint reads

$$\dot{H}_Y^* = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}_Y^*) = H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - Y). \tag{2.1.2}$$

By an explicit computation the equation

$$\dot{H}_Y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_Y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{2.1.3}$$

has the solutions

$$\psi_j(k, x) = e^{ik|x - y_j|}, \qquad \operatorname{Im} k > 0, \quad y_j \in Y, \quad j = 1, \ldots, N, \tag{2.1.4}$$

which therefore span the deficiency subspace of $\dot{H}_Y$. Thus $\dot{H}_Y$ has deficiency indices (N, N), and hence all self-adjoint extensions of $\dot{H}_Y$ are given by an N^2-parameter family of self-adjoint operators. Here we restrict ourselves to the case of so-called separated boundary conditions at each point y_j, $j = 1, \ldots, N$. Thus we introduce the following N-parameter family of closed extensions of $\dot{H}_Y$

$$-\Delta_{\alpha,Y} = -\frac{d^2}{dx^2},$$

$$\mathscr{D}(-\Delta_{\alpha,Y}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - Y) | g'(y_j+) - g'(y_j-) = \alpha_j g(y_j), \\ j = 1, \ldots, N\},$$

$$\alpha = (\alpha_1, \ldots, \alpha_N), \quad -\infty < \alpha_j \leq \infty, \quad j = 1, \ldots, N. \quad (2.1.5)$$

A simple integration by parts proves that $-\Delta_{\alpha,Y}$ is symmetric. Moreover, since $\dot{H}_Y$ has deficiency indices (N, N) and the N boundary conditions in (2.1.5) are symmetric and linearly independent, $-\Delta_{\alpha,Y}$ is self-adjoint ([158], Theorem XII. 4.30). The special case $\alpha = 0$ (i.e., $\alpha_j = 0, j = 1, \ldots, N$) again leads to the kinetic energy operator $-\Delta$ on $H^{2,2}(\mathbb{R})$. The case $\alpha_{j_0} = \infty$ for some j_0 leads to a Dirichlet boundary condition at the point y_{j_0} (i.e., $g(y_{j_0}+) = g(y_{j_0}-) = 0$). By definition $-\Delta_{\alpha,Y}$ describes N δ-interactions of strength α_j centered at the points $y_j \in Y, j = 1, \ldots, N$.

We now summarize some of the basic properties of $-\Delta_{\alpha,Y}$:

Theorem 2.1.1. *Let $\alpha_j \neq 0, j = 1, \ldots, N$. Then the resolvent of $-\Delta_{\alpha,Y}$ is given by*

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} (\overline{G_k(\cdot - y_{j'})}, \cdot) G_k(\cdot - y_j),$$

$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0, \quad -\infty < \alpha_j \leq \infty, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad (2.1.6)$$

where

$$\Gamma_{\alpha,Y}(k) = -[\alpha_j^{-1}\delta_{jj'} + G_k(y_j - y_{j'})]_{j,j'=1}^{N}. \quad (2.1.7)$$

Proof. One can follow the corresponding proof of Theorem I.3.1.2. Let $g \in L^2(\mathbb{R})$ and define

$$h_\alpha(x) = (i/2k) \int_{\mathbb{R}} dx'\, e^{ik|x-x'|} g(x')$$

$$- (1/4k^2) \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} \int_{\mathbb{R}} dx'\, e^{ik|x'-y_{j'}|} g(x') e^{ik|x-y_j|}, \qquad \operatorname{Im} k > 0, \quad (2.1.8)$$

where k is chosen such that $\det[\Gamma_{\alpha,Y}(k)] \neq 0$. Then, obviously, $h_\alpha \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - Y)$ and by inspection

$$h_\alpha'(y_j+) - h_\alpha'(y_j-) = \alpha_j h_\alpha(y_j), \qquad j = 1, \ldots, N. \quad (2.1.9)$$

Thus $h_\alpha \in \mathscr{D}(-\Delta_{\alpha,Y})$ and

$$((-\Delta_{\alpha,Y} - k^2)h_\alpha)(x) = -h_\alpha''(x) - k^2 h_\alpha(x) = g(x), \qquad x \in \mathbb{R} - Y, \quad (2.1.10)$$

which proves (2.1.6). The explicit structure of (2.1.6) then shows that $(-\Delta_{\alpha,Y} - k^2)^{-1}$ has a first-order pole in $\operatorname{Im} k > 0$ iff $\det[\Gamma_{\alpha,Y}(k)] = 0$. ∎

If some of the α_j equal zero, one extends the definition of $-\Delta_{\alpha,Y}$ as usual by deleting the corresponding lines and rows in $\Gamma_{\alpha,Y}(k)$.

Locality and additional domain properties of $-\Delta_{\alpha,Y}$ are described in

Theorem 2.1.2. *Let $-\infty < \alpha_j \leq \infty$, $\alpha_j \neq 0$, $y_j \in Y$, $j = 1, \ldots, N$. Then the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}\phi_k(y_{j'})G_k(x - y_j), \tag{2.1.11}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ and $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$. The decomposition (2.1.11) is unique and with $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ of this form we obtain

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{2.1.12}$$

Next let $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ and suppose that $\psi = 0$ in an open set $U \subseteq \mathbb{R}$. Then $-\Delta_{\alpha,Y}\psi = 0$ in U.

Proof. Since one can follow the proof of Theorem 1.1.3 step by step, we omit the details. ∎

It remains to discuss spectral properties of $-\Delta_{\alpha,Y}$:

Theorem 2.1.3. *Let $\alpha_j \neq 0$, $y_j \in Y$, $j = 1, \ldots, N$. Assume that at most one $\alpha_{j_0} = \infty$. Then $-\Delta_{\alpha,Y}$ has at most N eigenvalues which are all negative and simple. If $\alpha_j = \infty$ for at least two different values $j \in \{1, \ldots, N\}$, then $-\Delta_{\alpha,Y}$ has at most N negative eigenvalues (counting multiplicity) and infinitely many eigenvalues embedded in $[0, \infty)$ accumulating at ∞. In particular,*

$$k^2 \in \sigma_p(-\Delta_{\alpha,Y}) \cap (-\infty, 0) \quad \text{iff} \quad \det[\Gamma_{\alpha,Y}(k)] = 0, \qquad \operatorname{Im} k > 0, \tag{2.1.13}$$

and the multiplicity of the eigenvalue $k^2 < 0$ equals the multiplicity of the eigenvalue zero of the matrix $\Gamma_{\alpha,Y}(k)$. Moreover, if $E_0 = k_0^2 < 0$ is an eigenvalue of $-\Delta_{\alpha,Y}$, the corresponding eigenfunctions are of the form

$$\psi_0(x) = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \qquad \operatorname{Im} k_0 > 0, \tag{2.1.14}$$

where $(c_1, \ldots, c_N)$ are eigenvectors of the matrix $\Gamma_{\alpha,Y}(k_0)$ to the eigenvalue zero. If $-\Delta_{\alpha,Y}$ has a ground state it is nondegenerate and the corresponding eigenfunction can be chosen to be strictly positive (i.e., the associated eigenvector $(c_1, \ldots, c_N)$ fulfills $c_j > 0, j = 1, \ldots, N$).

The remaining part of the spectrum is absolutely continuous and covers the nonnegative real line

$$\sigma_{\mathrm{ess}}(-\Delta_{\alpha,Y}) = \sigma_{\mathrm{ac}}(-\Delta_{\alpha,Y}) = [0, \infty), \qquad \sigma_{\mathrm{sc}}(-\Delta_{\alpha,Y}) = \varnothing,$$
$$-\infty < \alpha_j \leq \infty, \quad j = 1, \ldots, N. \tag{2.1.15}$$

Proof. Since $\dot{H}_Y \geq 0$ and $\dot{H}_Y$ has deficiency indices (N, N), $-\Delta_{\alpha,Y}$ has at most N negative eigenvalues counting multiplicity ([494], p. 246). Relations (2.1.13) and (2.1.14) then follow as in Theorem 1.1.4 and all statements in (2.1.15) can be proved as in Theorem I.3.1.4. The remaining facts about the point spectrum are proved as follows: Without loss of generality assume

$$y_1 < y_2 < \cdots < y_N. \tag{2.1.16}$$

If all $|\alpha_j| < \infty, j = 1, \ldots, N$, one can follow [106] and define

$$\psi_k(x) = \begin{cases} a_1 e^{ikx} + b_1 e^{-ikx}, & x \le y_1, \\ a_{m+1} e^{ikx} + b_{m+1} e^{-ikx}, & y_m \le x \le y_{m+1}, \quad 1 \le m \le N-1, \\ a_{N+1} e^{ikx} + b_{N+1} e^{-ikx}, & x \ge y_N; \quad \operatorname{Im} k \ge 0, \quad k \ne 0, \end{cases} \tag{2.1.17}$$

where a_{m+1} and b_{m+1} are unique (nontrivial) solutions of

$$\begin{aligned} a_{m+1} e^{iky_m} + b_{m+1} e^{-iky_m} &= a_m e^{iky_m} + b_m e^{-iky_m}, \\ a_{m+1} e^{iky_m}[1 - (\alpha_m/ik)] - b_{m+1} e^{-iky_m}[1 + (\alpha_m/ik)] & \\ = a_m e^{iky_m} - b_m e^{-iky_m}, &\qquad 1 \le m \le N, \\ a_1 = a, \quad b_1 = b, \quad a, b \in \mathbb{R}. & \end{aligned} \tag{2.1.18}$$

Then $\psi_k(x)$ obeys

$$\psi_k(y_j+) = \psi_k(y_j-), \qquad \psi_k'(y_j+) - \psi_k'(y_j-) = \alpha_j \psi_k(y_j), \qquad j = 1, \ldots, N. \tag{2.1.19}$$

In addition, by the uniqueness of the coefficients $a_{m+1}, b_{m+1}, 1 \le m \le N$, ψ_k is the unique solution (up to multiplicative constants) of

$$-\psi_k''(x) = k^2 \psi_k(x), \qquad x \in \mathbb{R} - Y, \tag{2.1.20}$$

obeying the boundary conditions (2.1.19). If $k^2 > 0$, then $\psi_k \in L^2(\mathbb{R})$ iff $a = b = 0$, implying $\psi_k = 0$. Since the same argument (replace $e^{\pm ikx}$ by 1, x) applies for $k = 0$ we obtain $\sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0)$ in this case. For $k^2 < 0$, we get $a = 0$ and the above-mentioned uniqueness proves the simplicity of the eigenvalue. (Actually $k^2 < 0$ corresponds to an eigenvalue of $-\Delta_{\alpha,Y}$ iff $b_{N+1} = 0$.)

Next, consider the case where precisely one of the α_j say $\alpha_{j_0} = \infty$ and $N \ge 2$ (for $N = 1$, cf. Theorem I.3.1.4). Then the boundary condition at y_{j_0} reduces to $g(y_{j_0}\pm) = 0$ (with no conditions on $g'(y_{j_0}\pm)$), i.e., it becomes a Dirichlet boundary condition and hence divides $\mathbb{R}$ into two independent intervals $(-\infty, y_{j_0})$ and (y_{j_0}, ∞). It suffices to consider (y_{j_0}, ∞). If necessary, we renumber $y_{j_0} < y_{j_0+1} < \cdots < y_N$ to get $\tilde{y}_1 < \tilde{y}_2 < \cdots < \tilde{y}_M$ for some $M \le N$. Then we introduce

$$\psi_k(x) = \begin{cases} \tilde{a} k^{-1} \sin[k(x - \tilde{y}_1)], & \tilde{y}_1 < x < \tilde{y}_2, \\ \tilde{a}_{m+1} e^{ikx} + \tilde{b}_{m+1} e^{-ikx}, & \tilde{y}_m \le x \le \tilde{y}_{m+1}, \quad 2 \le m \le M-1, \\ \tilde{a}_{M+1} e^{ikx} + \tilde{b}_{M+1} e^{-ikx}, & x \ge \tilde{y}_M; \quad \operatorname{Im} k \ge 0, \quad k \ne 0, \end{cases} \tag{2.1.21}$$

where now $\tilde{a}_{m+1}$ and $\tilde{b}_{m+1}$ are unique (nontrivial) solutions of

$$\begin{aligned} \tilde{a}_{m+1} e^{ik\tilde{y}_m} + \tilde{b}_{m+1} e^{-ik\tilde{y}_m} &= \tilde{a}_m e^{ik\tilde{y}_m} + \tilde{b}_m e^{-ik\tilde{y}_m}, \\ \tilde{a}_{m+1} e^{ik\tilde{y}_m}[ik - \alpha_m] - \tilde{b}_{m+1} e^{-ik\tilde{y}_m}[ik + \alpha_m] &= ik\tilde{a}_m e^{ik\tilde{y}_m} - ik\tilde{b}_m e^{-ik\tilde{y}_m}, \quad 3 \le m \le M, \\ \tilde{a}_3 e^{ik\tilde{y}_2} + \tilde{b}_3 e^{-ik\tilde{y}_2} &= \tilde{a} k^{-1} \sin[k(\tilde{y}_2 - \tilde{y}_1)], \\ \tilde{a}_3 e^{ik\tilde{y}_2}(ik - \alpha_2) - \tilde{b}_3 e^{-ik\tilde{y}_2}(ik + \alpha_2) &= \tilde{a} \cos[k(\tilde{y}_2 - \tilde{y}_1)]. \end{aligned} \tag{2.1.22}$$

Then $\psi_k \in AC_{\text{loc}}((\tilde{y}_1, \infty))$, $\psi_k' \in AC_{\text{loc}}((\tilde{y}_1, \infty) - \{\tilde{y}_2, \ldots, \tilde{y}_M\})$,

$$\psi_k(\tilde{y}_1+) = 0,$$

$$\psi_k(\tilde{y}_1+) = \psi_k(\tilde{y}_1-), \qquad \psi_k'(\tilde{y}_j+) - \psi_k'(\tilde{y}_j-) = \alpha_j \psi_k(\tilde{y}_j), \qquad j = 2, \ldots, M, \tag{2.1.23}$$

and (up to multiplicative constants) ψ_k uniquely solves

$$-\psi_k''(x) = k^2\psi_k(x), \qquad \tilde{y}_1 < x < \infty, \quad x \neq \tilde{y}_2, \ldots, \tilde{y}_M, \tag{2.1.24}$$

and the boundary conditions (2.1.23). If $k^2 > 0$, then $\psi_k \in L^2((\tilde{y}_1, \infty))$ would imply $\tilde{a}_{M+1} = \tilde{b}_{M+1} = 0$ and hence $\psi_k = 0$. The same argument works for $k = 0$. Since an analogous construction works in the interval $(-\infty, y_{j_0})$ and $-\Delta_{\alpha,Y}$ is the direct sum of the corresponding operators in $L^2((-\infty, y_{j_0}))$ and $L^2((y_{j_0}, \infty))$, we also obtain $\sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0)$ in this case. Simplicity of negative eigenvalues then follows from the above-mentioned uniqueness of ψ_k.

It remains to show that if $\alpha_j = \infty$ for at least two different values of $j \in \{1, \ldots, N\}$, then $-\Delta_{\alpha,Y}$ has infinitely many eigenvalues embedded in $[0, \infty)$ accumulating at ∞. Let, e.g., $\alpha_{j_0} = \alpha_{j_1} = \infty$, $y_{j_0} < y_{j_1}$. Then by the arguments above, $-\Delta_{\alpha,Y}$ can be written as a direct sum of the corresponding operators in $L^2((-\infty, y_{j_0}))$, $L^2((y_{j_0}, y_{j_1}))$, and $L^2((y_{j_1}, \infty))$ with Dirichlet boundary conditions at y_{j_0} and y_{j_1}, respectively. But since (y_{j_0}, y_{j_1}) is a bounded interval, the essential spectrum of the corresponding operator in $L^2((y_{j_0}, y_{j_1}))$ is empty implying that its discrete spectrum accumulates at ∞. All properties of the ground state are shown as in Theorem 1.1.4 (cf. Appendix F for a detailed treatment). ∎

As in the one-center case the pole structure in (2.1.6) determines bound states as well as resonances of $-\Delta_{\alpha,Y}$. In particular, any solution k_1 of $\det[\Gamma_{\alpha,Y}(k_1)] = 0$ with $\operatorname{Im} k_1 < 0$ defines a resonance of $-\Delta_{\alpha,Y}$ whose multiplicity by definition coincides with the multiplicity of the zero of $\det[\Gamma_{\alpha,Y}(k)]$ at $k = k_1$. At $k = 0$ one has to investigate directly $[\Gamma_{\alpha,Y}(k)]^{-1}$ as $k \to 0$ since $\Gamma_{\alpha,Y}(0)$ does not exist.

Similar to Sect. I.3.1 we remark that for $\alpha_j \in \mathbb{R}$, $j = 1, \ldots, N$, $-\Delta_{\alpha,Y}$ can be obtained from the theory of quadratic forms as follows: The form

$$\begin{aligned} &Q_{\alpha,Y}(g, h) = (g', h') + \sum_{j=1}^{N} \alpha_j \overline{g(y_j)} h(y_j), \\ &\mathscr{D}(Q_{\alpha,Y}) = H^{2,1}(\mathbb{R}), \quad \alpha_j \in \mathbb{R}, \qquad y_j \in Y, \quad j = 1, \ldots, N, \end{aligned} \tag{2.1.25}$$

is densely defined, semibounded, and closed and the unique self-adjoint operator associated with $Q_{\alpha,Y}$ is given by $-\Delta_{\alpha,Y}$ (cf. [512]).

Finally, we present a more detailed discussion of the two-center δ-interaction: Fix $\alpha_1, \alpha_2 \in \mathbb{R} - \{0\}$, $y_1, y_2 \in \mathbb{R}$. Then

$$\Gamma_{\alpha,Y}(k) = -\begin{bmatrix} \alpha_1^{-1} + (i/2k) & (i/2k)e^{ik|y_2-y_1|} \\ (i/2k)e^{ik|y_2-y_1|} & \alpha_2^{-1} + (i/2k) \end{bmatrix}, \qquad k \in \mathbb{C} - \{0\}, \tag{2.1.26}$$

and hence

$$\begin{aligned} [\Gamma_{\alpha,Y}(k)]^{-1} = &-\{[\alpha_1^{-1} + (i/2k)][\alpha_2^{-1} + (i/2k)] \\ &+ (e^{2ik|y_2-y_1|}/4k^2)\}^{-1} \begin{bmatrix} \alpha_2^{-1} + (i/2k) & e^{ik|y_2-y_1|}/2ik \\ e^{ik|y_2-y_1|}/2ik & \alpha_1^{-1} + (i/2k) \end{bmatrix} \end{aligned} \tag{2.1.27}$$

as long as $\det[\Gamma_{\alpha,Y}(k)] \neq 0$. For $k \to 0$ we obtain

$$\begin{aligned} [\Gamma_{\alpha,Y}(k)]^{-1} \underset{k\to 0}{=} -[\alpha_1^{-1} + \alpha_2^{-1} + |y_2 - y_1| + O(k)]^{-1} \left\{ \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + O(k) \right\}, \\ \alpha_1^{-1} + \alpha_2^{-1} + |y_2 - y_1| \neq 0. \end{aligned} \tag{2.1.28}$$

In fact, for $\alpha_1^{-1} + \alpha_2^{-1} + |y_2 - y_1| \neq 0$ one can easily show that the first-order pole $i/2k$ in G_k actually cancels in the resolvent (2.1.6) of $-\Delta_{\alpha,Y}$.

The case $\alpha_1^{-1} + \alpha_2^{-1} + |y_2 - y_1| = 0$ implies a zero-energy resonance of $-\Delta_{\alpha,Y}$ as can be seen as follows. Let $c_1 \neq 0$ and assume without loss of generality $|\alpha_1| < \infty$ and $y_1 < y_2$. Define

$$\psi_0(x) = \begin{cases} c_1, & x \le y_1, \\ c_2 + c_3 x, & y_1 \le x \le y_2, \\ c_4, & x \ge y_2, \end{cases} \tag{2.1.29}$$

for appropriate constants $c_m \in \mathbb{C}$, $m = 1, \ldots, 4$. Then ψ_0 fulfills

$$\psi_0(y_j+) = \psi_0(y_j-), \qquad \psi_0'(y_j+) - \psi_0'(y_j-) = \alpha_j \psi_0(y_j), \qquad j = 1, 2, \tag{2.1.30}$$

if and only if

$$\alpha_1^{-1} + \alpha_2^{-1} + |y_2 - y_1| = 0 \tag{2.1.31}$$

in which case

$$c_2 = (1 - \alpha_1 y_1)c_1, \qquad c_3 = \alpha_1 c_1, \qquad c_4 = -(\alpha_1/\alpha_2)c_1 \tag{2.1.32}$$

(the case $\alpha_2 = \infty$, i.e., $c_4 = 0$, is included).

In general, the eigenvalues and resonances of $-\Delta_{\alpha,Y}$ are given by the equation

$$\det[\Gamma_{\alpha,Y}(k)] = -[\alpha_1^{-1} + (i/2k)][\alpha_2^{-1} + (i/2k)] - (e^{2ik|y_2-y_1|}/4k^2) = 0. \tag{2.1.33}$$

In the Dirichlet case $\alpha_1 = \alpha_2 = \infty$ we get, in particular,

$$(e^{2ik|y_2-y_1|} - 1)/4k^2 = 0 \tag{2.1.34}$$

and hence infinitely many positive eigenvalues E_n, $n = 1, 2, \ldots$, accumulating at ∞ (cf. Theorem 2.1.3)

$$E_n = k_n^2 = [\pi n/|y_2 - y_1|]^2, \qquad n = 1, 2, \ldots. \tag{2.1.35}$$

II.2.2 Approximations by Means of Local Scaled Short-Range Interactions

We now intend to generalize Sect. I.3.2 to finitely many δ-interactions. For this purpose we introduce real-valued potentials $V_j \in L^1(\mathbb{R})$, $j = 1, \ldots, N$, and define

$$v_j(x) = |V_j(x)|^{1/2}, \qquad u_j(x) = |V_j(x)|^{1/2}\,\mathrm{sgn}[V_j(x)], \qquad j = 1, \ldots, N. \tag{2.2.1}$$

In addition, we consider

$$\begin{gathered} \tilde{B}_\varepsilon(k)\colon L^2(\mathbb{R})^N \to L^2(\mathbb{R})^N, \\ [\tilde{B}_\varepsilon(k)(g_1, \ldots, g_N)]_j = \sum_{j'=1}^{N} \tilde{B}_{\varepsilon,jj'}(k) g_{j'}, \qquad g_j \in L^2(\mathbb{R}), \end{gathered} \tag{2.2.2}$$

where

$$\tilde{B}_{\varepsilon,jj'}(k) = \lambda_j(\varepsilon)\tilde{u}_j G_k \tilde{v}_{j'}, \qquad \varepsilon > 0, \quad \operatorname{Im} k > 0, \quad j, j' = 1, \ldots, N, \quad (2.2.3)$$

and $\lambda_j(\cdot)$ are real-analytic near the origin with $\lambda_j(0) = 0$, and

$$\tilde{u}_j(x) = u_j(x - \varepsilon^{-1}y_j), \quad \tilde{v}_j(x) = v_j(x - \varepsilon^{-1}y_j), \qquad \varepsilon > 0, \quad y_j \in Y,$$
$$j = 1, \ldots, N. \quad (2.2.4)$$

By Lemma I.3.2.1, $\tilde{B}_{\varepsilon,jj'}(k), j, j' = 1, \ldots, N$, extend to Hilbert–Schmidt operators for $\operatorname{Im} k \geq 0$, $k \neq 0$.

Using the theory of quadratic forms (cf. Appendix B) we then define the Hamiltonian $H_Y(\varepsilon)$ in $L^2(\mathbb{R})$

$$H_Y(\varepsilon) = -\Delta \dotplus \sum_{j=1}^{N} \lambda_j(\varepsilon) V_j(\cdot - \varepsilon^{-1}y_j), \qquad \varepsilon > 0, \quad Y \subset \mathbb{R}, \qquad (2.2.5)$$

with resolvent given by

$$[H_Y(\varepsilon) - k^2]^{-1} = G_k - \sum_{j,j'=1}^{N} (G_k\tilde{v}_j)[1 + \tilde{B}_\varepsilon(k)]^{-1}_{jj'}(\tilde{u}_{j'}G_k),$$
$$\varepsilon > 0, \quad k^2 \in \rho(H_Y(\varepsilon)), \quad \operatorname{Im} k > 0. \quad (2.2.6)$$

Next we use the unitary scaling group U_ε of (I.3.2.13) to define the Hamiltonian $H_{\varepsilon,Y}$ in $L^2(\mathbb{R})$

$$H_{\varepsilon,Y} = \varepsilon^{-2}U_\varepsilon H_Y(\varepsilon)U_\varepsilon^{-1} = -\Delta \dotplus \varepsilon^{-2}\sum_{j=1}^{N} \lambda_j(\varepsilon) V_j((\cdot - y_j)/\varepsilon),$$
$$\varepsilon > 0, \quad Y \subset \mathbb{R}. \quad (2.2.7)$$

Since we are interested in the limit $\varepsilon \downarrow 0$ of $H_{\varepsilon,Y}$ we introduce Hilbert–Schmidt operators $A_{\varepsilon,j}(k)$, $B_{\varepsilon,jj'}(k)$, $C_{\varepsilon,j}(k)$, $\varepsilon > 0$, with integral kernels

$$A_{\varepsilon,j}(k, x, x') = G_k(x - y_j - \varepsilon x')v_j(x'), \qquad \operatorname{Im} k > 0, \qquad (2.2.8)$$

$$B_{\varepsilon,jj'}(k, x, x') = \varepsilon^{-1}\lambda_j(\varepsilon)u_j(x)G_k(\varepsilon(x - x') + y_j - y_{j'})v_{j'}(x'),$$
$$\operatorname{Im} k \geq 0, \quad (2.2.9)$$

$$C_{\varepsilon,j}(k, x, x') = u_j(x)G_k(\varepsilon x + y_j - x'), \qquad \operatorname{Im} k > 0. \qquad (2.2.10)$$

Then (I.3.2.18) and suitable translations imply

$$(H_{\varepsilon,Y} - k^2)^{-1} = \varepsilon^2 U_\varepsilon[H_Y(\varepsilon) - (\varepsilon k)^2]^{-1}U_\varepsilon^{-1}$$
$$= G_k - \varepsilon^{-1}\sum_{j,j'=1}^{N} A_{\varepsilon,j}(k)[1 + B_\varepsilon(k)]^{-1}_{jj'}\lambda_{j'}(\varepsilon)C_{\varepsilon,j'}(k),$$
$$\varepsilon > 0, \quad k^2 \in \rho(H_{\varepsilon,Y}), \quad \operatorname{Im} k > 0, \quad Y \subset \mathbb{R}. \quad (2.2.11)$$

Again we have

Lemma 2.2.1. *Define rank-one operators $A_j(k)$, $B_{jj'}(k)$, $C_j(k)$, $j, j' = 1, \ldots, N$, through their integral kernels*

$$A_j(k, x, x') = G_k(x - y_j)v_j(x'), \qquad \text{Im } k > 0, \tag{2.2.12}$$

$$B_{jj'}(k, x, x') = \lambda_j'(0)G_k(y_j - y_{j'})u_j(x)v_{j'}(x'), \qquad \text{Im } k \geq 0, \quad k \neq 0, \tag{2.1.13}$$

$$C_j(k, x, x') = u_j(x)G_k(y_j - x'), \qquad \text{Im } k > 0. \tag{2.2.14}$$

Then, for fixed k, Im $k > 0$, $A_{\varepsilon, j}(k)$, $B_{\varepsilon, jj'}(k)$, $C_{\varepsilon, j}(k)$ *converge in Hilbert–Schmidt norm to* $A_j(k)$, $B_{jj'}(k)$, $C_j(k)$, $j, j' = 1, \ldots, N$, *respectively, as* $\varepsilon \downarrow 0$.

PROOF. Identical to that of Lemma I.3.2.2. ■

Thus we get our main result

Theorem 2.2.2. *Suppose* $V_j \in L^1(\mathbb{R})$, $j = 1, \ldots, N$, *are real-valued and* $Y \subset \mathbb{R}$. *Then, as* $\varepsilon \downarrow 0$, $H_{\varepsilon, Y}$ *converges to* $-\Delta_{\alpha, Y}$ *in norm resolvent sense, i.e., if* $k^2 \in \rho(-\Delta_{\alpha, Y})$, *then*

$$\underset{\varepsilon \downarrow 0}{\text{n-lim}}\, (H_{\varepsilon, Y} - k^2)^{-1} = (-\Delta_{\alpha, Y} - k^2)^{-1}, \qquad Y \subset \mathbb{R}, \tag{2.2.15}$$

where

$$\alpha_j = \lambda_j'(0) \int_{\mathbb{R}} dx\, V_j(x), \qquad j = 1, \ldots, N. \tag{2.2.16}$$

PROOF. From (2.2.11) and Lemma 2.2.1 we obtain

$$\underset{\varepsilon \downarrow 0}{\text{n-lim}}\, (H_{\varepsilon, Y} - k^2)^{-1} = G_k - \sum_{j, j'=1}^{N} A_j(k)[1 + B(k)]_{jj'}^{-1} \lambda_{j'}'(0) C_{j'}(k),$$
$$k^2 \in \mathbb{C} - \mathbb{R}, \quad \text{Im } k > 0, \tag{2.2.17}$$

where $B(k)$ is defined by

$$\begin{aligned} &B(k)\colon L^2(\mathbb{R})^N \to L^2(\mathbb{R})^N, \qquad \text{Im } k \geq 0, \quad k \neq 0, \\ &[B(k)(g_1, \ldots, g_N)]_j = \sum_{j'=1}^{N} B_{jj'}(k) g_{j'}, \qquad g_j \in L^2(\mathbb{R}), \quad j = 1, \ldots, N. \end{aligned} \tag{2.2.18}$$

But

$$B_{jj'}(k) = \lambda'(0) G_k(y_j - y_{j'})(v_{j'}, \cdot)u_j \tag{2.2.19}$$

implies

$$[1 + B(k)]_{jj'}^{-1} = 1\delta_{jj'} - \lambda_j'(0) \sum_{m=1}^{N} G_k(y_j - y_m)[\hat{\Gamma}_{\alpha, Y}(k)]_{mj'}^{-1}(v_{j'}, \cdot)u_j, \tag{2.2.20}$$

where

$$\hat{\Gamma}_{\alpha, Y}(k) = [\delta_{jj'} + \lambda_j'(0)(v_j, u_j)G_k(y_j - y_{j'})]_{j, j'=1}^{N}, \qquad \text{Im } k > 0. \tag{2.2.21}$$

If $\lambda_j'(0)(v_j, u_j) \neq 0$ for all $j = 1, \ldots, N$, then a comparison with (2.1.7) shows that

$$[\hat{\Gamma}_{\alpha, Y}(k)]_{jj'}^{-1} \lambda_{j'}'(0)(v_{j'}, u_{j'}) = -[\Gamma_{\alpha, Y}(k)]_{jj'}^{-1}, \alpha_j = \lambda_j'(0)(v_j, u_j), \quad j, j' = 1, \ldots, N, \tag{2.2.22}$$

which by (2.1.6) completes the proof after inserting (2.2.22), (2.2.12), and (2.2.14) into (2.2.17). If, e.g., $\lambda'_{j_0}(0)(v_{j_0}, u_{j_0}) = 0$ for some j_0, then insertion of (2.2.22), (2.2.12), and (2.2.14) into (2.2.17) shows that all terms with $j = j_0$ or $j' = j_0$ in (2.2.17) are zero and hence disappear on the right-hand side of (2.2.17). ∎

Again $H_{\varepsilon,Y}$ converges to $-\Delta$ as $\varepsilon \downarrow 0$ if and only if $\lambda'_j(0) \int_{\mathbb{R}} dx\ V_j(x) = 0$ for all $j = 1, \ldots, N$ and similarly to the one-center case the above approximation scheme automatically yields δ-interactions at the points $y_1, \ldots, y_N$ with finite strengths $\alpha_1, \ldots, \alpha_N$. Moreover, the above proof immediately extends to the case of nonreal $\lambda_j(\varepsilon)$ to yield complex point interactions.

Formulas (2.2.17), (2.2.20), and (2.2.22) also show that bound states (resp. resonances) of $-\Delta_{\alpha,Y}$ are given by the zeros of the Fredholm determinant $\det[1 + B(k)]$ in the upper (resp. lower) k half-plane.

II.2.3 Convergence of Eigenvalues and Resonances

Having proved norm resolvent convergence of $H_{\varepsilon,Y}$ to $-\Delta_{\alpha,Y}$ as $\varepsilon \downarrow 0$ in the preceding section, we now extend this analysis to include a detailed description of how the corresponding eigenvalues and resonances of $H_{\varepsilon,Y}$ converge to those of $-\Delta_{\alpha,Y}$ in the same limit. On the basis of Theorem B.1(b) we first state that

$$\sigma_{\text{ess}}(H_{\varepsilon,Y}) = \sigma_{\text{ess}}(H_Y(\varepsilon)) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad \varepsilon > 0, \quad Y \subset \mathbb{R}. \tag{2.3.1}$$

By Theorem 2.1.3 this continues to hold at $\varepsilon = 0$

$$\sigma_{\text{ess}}(-\Delta_{\alpha,Y}) = \sigma_{\text{ess}}(-\Delta) = [0, \infty), \qquad -\infty < \alpha_j \le \infty, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{2.3.2}$$

For the discrete spectrum of $H_{\varepsilon,Y}$ a detailed study of $B_\varepsilon(k)$ yields

Theorem 2.3.1. *Let $Y \subset \mathbb{R}$, $y_j \in Y$, and suppose that $V_j \in L^1(\mathbb{R})$, $j = 1, \ldots, N$, are real-valued and have compact support.*

(a) *If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,Y} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,Y})$, *such that* $-\Delta_{\alpha,Y}$ *has* $1 \le M \le N$ *(necessarily simple) negative eigenvalues* $E_m = k_m^2 < 0$, $m = 1, \ldots, M$, *then, for* $\varepsilon > 0$ *small enough,* $H_{\varepsilon,Y}$ *has* M *simple eigenvalues* $E_{\varepsilon,m} = k_{\varepsilon,m}^2 < 0$ *which are analytic in* ε *near* $\varepsilon = 0$, *and*

$$k_{\varepsilon,m} = i\sqrt{-E_{\varepsilon,m}} = k_m + O(\varepsilon), \qquad m = 1, \ldots, M. \tag{2.3.3}$$

Moreover, $E_{\varepsilon,m}$ *are the only eigenvalues of* $H_{\varepsilon,Y}$ *near* E_m, $m = 1, \ldots, M$.

(b) *If* $\text{n-lim}_{\varepsilon\downarrow 0}(H_{\varepsilon,Y} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1}$, $k^2 \in \rho(-\Delta_{\alpha,Y})$, *such that* $-\Delta_{\alpha,Y}$ *has no negative eigenvalues, then all negative eigenvalues of* $H_{\varepsilon,Y}$ *tend to zero, i.e., are absorbed into the essential spectrum as* $\varepsilon \downarrow 0$.

PROOF. By Theorem B.1(c) any negative eigenvalue $E_\varepsilon = k_\varepsilon^2 < 0$ of $H_{\varepsilon,Y}$ is determined through solutions of

$$B_\varepsilon(k)\Phi_\varepsilon = -\Phi_\varepsilon, \qquad \Phi_\varepsilon \in L^2(\mathbb{R})^N, \quad \varepsilon > 0, \tag{2.3.4}$$

and the corresponding (geometric) multiplicities are preserved. In order to isolate the dominant term in $B_\varepsilon(k)$ we define the operator $\hat{B}_\varepsilon(k)$ in $L^2(\mathbb{R})^N$ with entries

$$\hat{B}_{\varepsilon,jj'}(k) = \varepsilon^{-1}\lambda_j(\varepsilon)(i/2k)e^{ik|y_j-y_{j'}|}(v_{j'},\ \cdot)u_j,$$

$$\varepsilon \geq 0, \quad k \in \mathbb{C} - \{0\}, \quad j, j' = 1, \ldots, N. \quad (2.3.5)$$

In particular, $\hat{B}_0(k) = B(k)$ (cf. (2.2.13) and (2.2.18)). Since V_j, $j = 1, \ldots, N$, have compact support, $B_\varepsilon(k)$ is analytic in (ε, k) for $|\varepsilon|$ small enough and $k \in \mathbb{C} - \{0\}$. Expanding $B_\varepsilon(k)$ with respect to ε yields

$$B_{\varepsilon,jj'}(k, x, x') = B_{jj'}(k, x, x') + \varepsilon\lambda_j''(\varepsilon\tilde{\theta}(\varepsilon))B_{jj'}(k, x, x')$$
$$- (\varepsilon/2)\lambda_j'(0)u_j(x)[(x - x')\operatorname{sgn}(y_j - y_{j'})e^{ik|y_j-y_{j'}+\varepsilon\theta(\varepsilon)(x-x')|}]v_{j'}(x'),$$
$$\varepsilon \geq 0, \quad k \in \mathbb{C} - \{0\}, \quad j, j' = 1, \ldots, N, \quad (2.3.6)$$

for appropriate $0 \leq \theta(\varepsilon), \tilde{\theta}(\varepsilon) \leq 1$, where we define $\operatorname{sgn}(0) = 1$. Thus

$$\|B_\varepsilon(k) - \hat{B}_\varepsilon(k)\| = O(\varepsilon) \quad (2.3.7)$$

uniformly in k if k varies in compact subsets of $\mathbb{C}$ and

$$\|B_\varepsilon(k)\| = O(|k|^{-1}) \quad \text{as } |k| \to \infty, \qquad \operatorname{Im} k \geq 0, \quad (2.3.8)$$

uniformly in ε, $|\varepsilon|$ small enough. Applying formula (I.3.3.11) then shows that for $|\varepsilon|$ small enough

$$\det[1 + B_\varepsilon(k)] = \det[1 + B_\varepsilon(k) - \hat{B}_\varepsilon(k)] \det\{1 + [1 + B_\varepsilon(k) - \hat{B}_\varepsilon(k)]^{-1}\hat{B}_\varepsilon(k)\} \quad (2.3.9)$$

vanishes for some $k \in \mathbb{C} - \{0\}$ if and only if

$$\det\{1 + [1 + B_\varepsilon(k) - \hat{B}_\varepsilon(k)]^{-1}\hat{B}_\varepsilon(k)\} \quad (2.3.10)$$

vanishes. Now assume that $\det[1 + B(k_m)] = 0$ for some k_m, $\operatorname{Im} k_m > 0$, or equivalently, suppose that $E_m = k_m^2 < 0$ is an eigenvalue of $-\Delta_{\alpha,Y}$. Then by the simplicity of E_m (cf. Theorem 2.1.3) and the analyticity of $B_\varepsilon(k)$, $\hat{B}_\varepsilon(k)$ in (ε, k) for $|\varepsilon|$ small enough and $k \in \mathbb{C} - \{0\}$, we infer by the implicit function theorem that in a neighborhood of k_m (2.3.10) has a unique and simple zero $k_{\varepsilon,m}$ analytic in ε near $\varepsilon = 0$ such that (2.3.3) holds. By Theorem B.1(c), $E_{\varepsilon,m} = k_{\varepsilon,m}^2 < 0$ corresponds to a simple eigenvalue of $H_{\varepsilon,Y}$. Since $H_{\varepsilon,Y}$ converges to $-\Delta_{\alpha,Y}$ in norm resolvent sense as $\varepsilon \downarrow 0$, remaining eigenvalues of $H_{\varepsilon,Y}$ are forced to converge to zero or to $-\infty$ as $\varepsilon \downarrow 0$. By (2.3.8) eigenvalues running to $-\infty$ are excluded. ■

The fact that no eigenvalues of $H_{\varepsilon,Y}$ run off to $-\infty$ as $\varepsilon \downarrow 0$ (due to the fact that $\lambda(\varepsilon) = O(\varepsilon)$ as $\varepsilon \downarrow 0$) is in sharp contrast to the corresponding case in three dimensions.

Concerning resonances we state

Theorem 2.3.2. *Let $Y \subset \mathbb{R}$, $y_j \in Y$, and assume that $V_j \in L^1(\mathbb{R})$, $j = 1, \ldots, N$, are real-valued and have compact support. Suppose that*

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\varepsilon,Y} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1}, \qquad k^2 \in \rho(-\Delta_{\alpha,Y}),$$

and that k_0, $\operatorname{Im} k_0 < 0$, is a resonance of $-\Delta_{\alpha,Y}$ with multiplicity M. Then, for $\varepsilon > 0$ small enough, there exist M (not necessarily distinct) resonances

$k_{l,\varepsilon}$, $\operatorname{Im} k_{l,\varepsilon} < 0$, $l = 1, \ldots, m$, of $H_{\varepsilon,Y}$ such that $k_{l,\varepsilon}$ have convergent Puiseux expansions in ε near $\varepsilon = 0$, i.e.,

$$k_{l,\varepsilon} = k_0 + h_l(\varepsilon^{1/m_l}) = k_0 + \sum_{r=1}^{\infty} a_{l,r}\varepsilon^{r/m_l}, \qquad l = 1, \ldots, m, \quad \sum_{l=1}^{m} m_l = M, \tag{2.3.11}$$

where h_l are analytic near the origin, $h_l(0) = 0$, $l = 1, \ldots, m$. In particular, $k_{l,\varepsilon}$ are the only resonances of $H_{\varepsilon,Y}$ near k_0.

PROOF. The only difference to the preceding proof concerns the fact that now the multiplicity of the zero of $\det[1 + B(k)]$ at $k = k_0$ is not necessarily one and hence yields Puiseux expansions for k_ε. ∎

II.2.4 Stationary Scattering Theory

In analogy to Sect. I.3.4 we first develop stationary scattering theory for δ-interactions and then show convergence of the scattering matrix corresponding to $H_{\varepsilon,Y}$ to that of $-\Delta_{\alpha,Y}$ as $\varepsilon \downarrow 0$. We start discussing stationary scattering theory for the pair $(-\Delta_{\alpha,Y}, -\Delta)$. Let

$$\begin{gathered}\Psi_{\alpha,Y}(k, \sigma, x) = e^{ik\sigma x} - (2ik)^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} e^{ik\sigma y_{j'}} e^{ik|x-y_j|}, \\ \det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k > 0, \quad \sigma = \pm 1, \quad -\infty < \alpha_j \leq \infty, \quad \alpha_j \neq 0, \quad y_j \in Y, \\ j = 1, \ldots, N, \quad x \in \mathbb{R},\end{gathered} \tag{2.4.1}$$

with $\Gamma_{\alpha,Y}(k)$ defined in (2.1.7). Then, for $k > 0$,

$$\begin{aligned} \Psi_{\alpha,Y}(k, \sigma, y_j+) &= \Psi_{\alpha,Y}(k, \sigma, y_j-), && j = 1, \ldots, N, \\ \Psi'_{\alpha,Y}(k, \sigma, y_j+) - \Psi'_{\alpha,Y}(k, \sigma, y_j-) &= \alpha_j \Psi_{\alpha,Y}(k, \sigma, y_j), && j = 1, \ldots, N, \\ -\Psi''_{\alpha,Y}(k, \sigma, x) &= k^2 \Psi_{\alpha,Y}(k, \sigma, x), && x \in \mathbb{R} - Y, \end{aligned} \tag{2.4.2}$$

$$\lim_{\varepsilon \downarrow 0} \lim_{x' \to \mp\infty} (2k/i) e^{\pm i(k+i\varepsilon)x'} [-\Delta_{\alpha,Y} - (k + i\varepsilon)^2]^{-1}(x, x') = \Psi_{\alpha,Y}(k, \pm 1, x), \qquad x \in \mathbb{R},$$

and hence $\Psi_{\alpha,Y}(k, \sigma)$ are generalized eigenfunctions associated with $-\Delta_{\alpha,Y}$ corresponding to left ($\sigma = +1$) and right incidence ($\sigma = -1$). The corresponding *transmission* and *reflection coefficients* from the left and right are defined by

$$\begin{aligned} \mathscr{T}^{\mathrm{l}}_{\alpha,Y}(k) &= \lim_{x \to +\infty} e^{-ikx} \Psi_{\alpha,Y}(k, +1, x) \\ &= \lim_{x \to -\infty} e^{ikx} \Psi_{\alpha,Y}(k, -1, x) = \mathscr{T}^{\mathrm{r}}_{\alpha,Y}(k), \\ \mathscr{R}^{\mathrm{l}}_{\alpha,Y}(k) &= \lim_{x \to -\infty} e^{ikx} [\Psi_{\alpha,Y}(k, +1, x) - e^{ikx}], \\ \mathscr{R}^{\mathrm{r}}_{\alpha,Y}(k) &= \lim_{x \to +\infty} e^{-ikx} [\Psi_{\alpha,Y}(k, -1, x) - e^{-ikx}], \end{aligned} \tag{2.4.3}$$

and thus

$$\mathscr{T}^{\mathrm{l}}_{\alpha,Y}(k) = 1 - (2ik)^{-1} \sum_{j,j'=1}^{N} e^{-iky_j}[\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} e^{iky_{j'}} = \mathscr{T}^{\mathrm{r}}_{\alpha,Y}(k), \tag{2.4.4}$$

$$\mathscr{R}^{\mathrm{l}}_{\alpha,Y}(k) = -(2ik)^{-1} \sum_{j,j'=1}^{N} e^{iky_j}[\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} e^{iky_{j'}}, \tag{2.4.5}$$

$$\mathscr{R}^{\mathrm{r}}_{\alpha,Y}(k) = -(2ik)^{-1} \sum_{j,j'=1}^{N} e^{-iky_j}[\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} e^{-iky_{j'}};$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k > 0, \quad -\infty < \alpha_j \leq \infty, \quad \alpha_j \neq 0, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{2.4.6}$$

The unitary on-shell scattering operator $\mathscr{S}_{\alpha,Y}(k)$ in $\mathbb{C}^2$ is then defined as usual by

$$\mathscr{S}_{\alpha,Y}(k) = \begin{bmatrix} \mathscr{T}^{\mathrm{l}}_{\alpha,Y}(k) & \mathscr{R}^{\mathrm{r}}_{\alpha,Y}(k) \\ \mathscr{R}^{\mathrm{l}}_{\alpha,Y}(k) & \mathscr{T}^{\mathrm{r}}_{\alpha,Y}(k) \end{bmatrix},$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k > 0, \quad -\infty \leq \alpha_j \leq \infty, \quad \alpha_j \neq 0, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{2.4.7}$$

Again $\mathscr{S}_{\alpha,Y}(k)$ has a meromorphic continuation in k to all of $\mathbb{C}$ such that poles of $\mathscr{S}_{\alpha,Y}(k)$ in $\mathbb{C}$-$\{0\}$ coincide with bound states or resonances of $-\Delta_{\alpha,Y}$.

For illustrations of transmission probabilities in the $N = 2$, 4, 8, and 20 center case with equally spaced δ-interactions (of mutual distance π), see Figure 40(b)–(e) [397] in Sect. III.2.3, p. 275.

Next we summarize stationary scattering theory associated with $H_{\varepsilon,Y}$. Let u_j, v_j be as in Sect. 2.2. We introduce in $L^2(\mathbb{R})^N$

$$\Phi^{\pm}_{\varepsilon,Y}(k,\sigma,x) = (\phi^{\pm}_{\varepsilon,y_1}(k,\sigma,x), \ldots, \phi^{\pm}_{\varepsilon,y_N}(k,\sigma,x)), \tag{2.4.8}$$

where

$$\begin{aligned} &\phi^{-}_{\varepsilon,y_j}(k,\sigma,x) = u_{\varepsilon,j}(x)e^{ik\sigma x}, \\ &\phi^{+}_{\varepsilon,y_j}(k,\sigma,x) = v_{\varepsilon,j}(x)e^{ik\sigma x}, \qquad \varepsilon > 0, \quad k \geq 0, \quad \sigma = \pm 1, \end{aligned} \tag{2.4.9}$$

and

$$u_{\varepsilon,j}(x) = u_j((x - y_j)/\varepsilon), \qquad v_{\varepsilon,j}(x) = v_j((x - y_j)/\varepsilon),$$
$$\varepsilon > 0, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{2.4.10}$$

The elements $t_{\varepsilon,jj'}(k)$, $j, j' = 1, \ldots, N$, in $L^2(\mathbb{R})$ of the transition operator $t_\varepsilon(k)$ in $L^2(\mathbb{R})^N$ are then defined by

$$t_{\varepsilon,jj'}(k) = \varepsilon^{-2}\lambda_{j'}(\varepsilon)[1 + \mathring{B}_\varepsilon(k)]^{-1}_{jj'},$$
$$\varepsilon > 0, \quad \operatorname{Im} k \geq 0, \quad k \neq 0, \quad k^2 \notin \mathscr{E}_\varepsilon, \quad j, j' = 1, \ldots, N, \tag{2.4.11}$$

where

$$\mathring{B}_\varepsilon(k)\colon L^2(\mathbb{R})^N \to L^2(\mathbb{R})^N,$$

$$[\mathring{B}_\varepsilon(k)(g_1, \ldots, g_N)]_j = \sum_{j'=1}^{N} \mathring{B}_{\varepsilon,jj'}(k) g_{j'}, \qquad g_j \in L^2(\mathbb{R}), \tag{2.4.12}$$

$$\mathring{B}_{\varepsilon,jj'}(k) = \varepsilon^{-2}\lambda_j(\varepsilon) u_{\varepsilon,j} G_k v_{\varepsilon,j'},$$
$$\varepsilon > 0, \quad \operatorname{Im} k \geq 0, \quad k \neq 0, \quad j, j' = 1, \ldots, N,$$

and

$$\mathscr{E}_\varepsilon = \{k^2 \in \mathbb{C} - \{0\} \mid B_\varepsilon(k)\Phi_\varepsilon = -\Phi_\varepsilon \text{ for some } \Phi_\varepsilon \in L^2(\mathbb{R})^N, \operatorname{Im} k \geq 0\}. \tag{2.4.13}$$

Here $B_\varepsilon(k)$ is defined as

$$\begin{aligned} &B_\varepsilon(k)\colon L^2(\mathbb{R})^N \to L^2(\mathbb{R})^N, \\ &[B_\varepsilon(k)(g_1, \ldots, g_N)]_j = \sum_{j'=1}^N B_{\varepsilon,jj'}(k) g_{j'}, \qquad g_j \in L^2(\mathbb{R}), \quad j = 1, \ldots, N, \end{aligned} \tag{2.4.14}$$

with $B_{\varepsilon,jj'}(k)$ given in (2.2.9). Again $\mathscr{E}_\varepsilon \cap (0, \infty) = \varnothing$ by Jost function techniques. The *on-shell scattering amplitude* $f_{\varepsilon,Y,\sigma\sigma'}(k)$ is then given by

$$\begin{aligned} f_{\varepsilon,Y,\sigma\sigma'}(k) &= (2ik)^{-1}(\Phi^+_{\varepsilon,Y}(k,\sigma), t_\varepsilon(k)\Phi^-_{\varepsilon,Y}(k,\sigma')) \\ &= (2ik)^{-1} \sum_{j,j'=1}^N (\phi^+_{\varepsilon,y_j}(k,\sigma), t_{\varepsilon,jj'}(k)\phi^-_{\varepsilon,y_{j'}}(k,\sigma')), \\ &\qquad \varepsilon, k > 0, \quad \sigma, \sigma' = \pm 1, \quad Y \subset \mathbb{R}. \end{aligned} \tag{2.4.15}$$

The unitary *on-shell scattering matrix* $S_{\varepsilon,Y}(k) = [S_{\varepsilon,Y,\sigma\sigma'}(k)]_{\sigma,\sigma'=\pm 1}$ in $\mathbb{C}^2$ then reads

$$S_{\varepsilon,Y,\sigma\sigma'}(k) = \delta_{\sigma\sigma'} + f_{\varepsilon,Y,\sigma\sigma'}(k), \qquad \varepsilon, k > 0, \quad \sigma, \sigma' = \pm 1, \quad Y \subset \mathbb{R}, \tag{2.4.16}$$

and the *transmission* and *reflection coefficients* corresponding to $H_{\varepsilon,Y}$ are defined by

$$\begin{aligned} &T^1_{\varepsilon,Y}(k) = S_{\varepsilon,Y,++}(k) = S_{\varepsilon,Y,--}(k) = T^r_{\varepsilon,Y}(k), \\ &R^1_{\varepsilon,Y}(k) = S_{\varepsilon,Y,-+}(k), \qquad R^r_{\varepsilon,Y}(k) = S_{\varepsilon,Y,+-}(k); \quad \varepsilon, k > 0, \quad Y \subset \mathbb{R}. \end{aligned} \tag{2.4.17}$$

Given the above notions we are in a position to describe in what sense $S_{\varepsilon,Y}(k)$ approaches $\mathscr{S}_{\alpha,Y}(k)$ as $\varepsilon \downarrow 0$:

Theorem 2.4.1. *Let $V_j \in L^1(\mathbb{R})$ be real-valued and let $\alpha_j = \lambda_j'(0)\int_{\mathbb{R}} dx\, V_j(x)$ and $y_j \in Y, j = 1, \ldots, N$. Then $S_{\varepsilon,Y}(k)$, $k > 0$, $\det[\Gamma_{\alpha,Y}(k)] \neq 0$ converges to $\mathscr{S}_{\alpha,Y}(k)$ as $\varepsilon \downarrow 0$. If, in addition, $V_j, j = 1, \ldots, N$, have compact support then $S_{\varepsilon,Y}(k)$ is analytic in ε near $\varepsilon = 0$ and we obtain the expansion*

$$\begin{aligned} &S_{\varepsilon,Y}(k) \underset{\varepsilon \to 0}{=} \mathscr{S}_{\alpha,Y}(k) + O(\varepsilon), \qquad k > 0, \\ &\alpha_j = \lambda_j'(0) \int_{\mathbb{R}} dx\, V_j(x), \qquad y_j \in Y, \quad j = 1, \ldots, N. \end{aligned} \tag{2.4.18}$$

PROOF. Let $V_j \in L^1(\mathbb{R}), j = 1, \ldots, N$. We first rewrite (2.4.15) to get

$$f_{\varepsilon,Y,\sigma\sigma'}(k) = (2ik)^{-1} \sum_{j,j'=1}^N \varepsilon^{-1}\lambda_{j'}(\varepsilon)(v_j e^{ik\sigma(\varepsilon x + y_j)}, U_\varepsilon^{-1} T_{y_j}[1 + \mathring{B}_\varepsilon(k)]^{-1}_{jj'} T_{-y_{j'}} U_\varepsilon u_{j'} e^{ik\sigma'(\varepsilon x' + y_{j'})}), \tag{2.4.19}$$

where x, x' are just integration variables and T_y, $y \in \mathbb{R}$, denotes the unitary translation group in $L^2(\mathbb{R})$, viz.

$$(T_y g)(x) = g(x + y), \qquad y \in \mathbb{R}, \quad g \in L^2(R). \tag{2.4.20}$$

Using

$$U_\varepsilon^{-1} T_{y_j} [1 + \mathring{B}_\varepsilon(k)]_{jj'}^{-1} T_{-y_{j'}} U_\varepsilon = [1 + B_\varepsilon(k)]_{jj'}^{-1}, \qquad j, j' = 1, \ldots, N. \quad (2.4.21)$$

we end up with

$$f_{\varepsilon, Y, \sigma\sigma'}(k) = (2ik)^{-1} \sum_{j,j'=1}^{N} \varepsilon^{-1} \lambda_{j'}(\varepsilon) (v_j e^{ik\sigma(\varepsilon x + y_j)}, [1 + B_\varepsilon(k)]_{jj'}^{-1} u_{j'} e^{ik\sigma'(\varepsilon x' + y_{j'})}). \quad (2.4.22)$$

Since by dominated convergence $v_j e^{ik\sigma\varepsilon(\cdot)}$, $u_j e^{ik\sigma'\varepsilon(\cdot)}$ are strongly continuous in ε, Lemma 2.2.1 immediately implies

$$\lim_{\varepsilon \downarrow 0} f_{\varepsilon, Y, \sigma\sigma'}(k) = (2ik)^{-1} \sum_{j,j'=1}^{N} \lambda'_{j'}(0) e^{-ik\sigma y_j} (v_j, [1 + B(k)]_{jj'}^{-1} u_{j'}) e^{ik\sigma' y_{j'}}. \quad (2.4.23)$$

Assuming $\lambda'_j(0)(v_j, u_j) \neq 0, j = 1, \ldots, N$, an application of (2.2.20) and (2.2.22) then shows

$$\lim_{\varepsilon \downarrow 0} f_{\varepsilon, Y, \sigma\sigma'} = -(2ik)^{-1} \sum_{j,j'=1}^{N} e^{-ik\sigma y_j} [\Gamma_{\alpha, Y}(k)]_{jj'}^{-1} e^{ik\sigma' y_{j'}}, \quad (2.4.24)$$

where $\Gamma_{\alpha, Y}(k)$ is given by (2.1.7) with

$$\alpha_j = \lambda'_j(0)(v_j, u_j), \qquad j = 1, \ldots, N. \quad (2.4.25)$$

If $\lambda'_{j_0}(0)(v_{j_0}, u_{j_0}) = 0$ for some j_0, then all terms with $j = j_0$ or $j' = j_0$ in (2.4.23) vanish and hence do not appear in (2.4.24). Thus $\Gamma_{\alpha, Y}(k)$ contains precisely those α_j which are nonvanishing. If $V_j, j = 1, \ldots, N$, have compact support, then analyticity of $B_\varepsilon(k)$ in ε for $|\varepsilon|$ small enough and fixed $k \in \mathbb{C}$, $k \neq 0$ (cf. Sect. 2.3), proves analyticity of $S_{\varepsilon, Y}(k)$, $k > 0$, near $\varepsilon = 0$. ■

Again $S_\varepsilon(k)$ converges to 1 as $\varepsilon \downarrow 0$ if and only if $\alpha_j = \lambda'_j(0) \int_{\mathbb{R}} dx\, V_j(x) = 0$, $j = 1, \ldots, N$, i.e., if all δ-interactions have vanishing strength and hence disappear.

Notes

Section II.2.1

This section represents an extended version of some of the results in [21]. Further theoretical background for the one-dimensional N-center case can be found in [106], [107], [226], [512]. For the two-center case, cf. [7], [121], [123], [190], [191], [395]. The relation between point interactions and self-adjoint extensions of $\dot{H}_Y$ different from $-\Delta_{\alpha, Y}$ (i.e., a choice of boundary conditions which connect different points in Y) has been considered in [129].

Sections II.2.2 and II.2.3

All results are taken from [21].

Section II.2.4

Scattering theory for N-center δ-interactions has been treated in [285] (see also [176]), [308], [316], [317], [379], [387], [397]. The first half of Theorem 2.4.1 has been derived in [379].

CHAPTER II.3

Finitely Many δ'-Interactions in One Dimension

In this chapter we extend the concepts of Ch. I.4 to finitely many δ'-interactions on the real line.

Let $N \in \mathbb{N}$ and introduce the set $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}$. We first introduce the closed and nonnegative minimal operator $\ddot{H}_Y$ in $L^2(\mathbb{R})$

$$\ddot{H}_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\ddot{H}_Y) = \{g \in H^{2,2}(\mathbb{R}) | g(y_j) = g'(y_j) = 0, j = 1, \ldots, N\}$$
$$= H_0^{2,2}(\mathbb{R} - Y) \tag{3.1}$$

whose adjoint is given by

$$\ddot{H}_Y^* = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\ddot{H}_Y^*) = H^{2,2}(\mathbb{R} - Y). \tag{3.2}$$

Since the equation

$$\ddot{H}_Y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\ddot{H}_Y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{3.3}$$

has the solutions

$$\psi_{j1}(k, x) = \begin{cases} e^{ik(x-y_j)}, & x > y_j, \\ 0, & x < y_j, \end{cases} \qquad \psi_{j2}(k, x) = \begin{cases} 0, & x > y_j, \\ e^{ik(y_j - x)}, & x < y_j, \end{cases}$$
$$\operatorname{Im} k > 0, \quad y_j \in Y, \quad j = 1, \ldots, N, \tag{3.4}$$

the operator $\ddot{H}_Y$ has deficiency indices $(2N, 2N)$. As in Ch. I.4 there exists an intermediate minimal operator $\dot{H}'_Y$ in $L^2(\mathbb{R})$ which is a proper symmetric extension of $\ddot{H}_Y$ (cf. the Notes to Ch. I.4). In fact, the closed operator $\dot{H}'_Y$

defined by

$$\dot{H}'_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}'_Y) = \{g \in H^{2,2}(\mathbb{R}) | g'(y_j) = 0,\ y_j \in Y, j = 1, \ldots, N\} \tag{3.5}$$

has deficiency indices (N, N) and hence is more convenient for the following treatment. We note that the adjoint of $\dot{H}'_Y$ is given by

$$\begin{gathered} \dot{H}'^{*}_Y = -\frac{d^2}{dx^2}, \\ \mathscr{D}(\dot{H}'^{*}_Y) = \{g \in H^{2,2}(\mathbb{R} - Y) | g'(y_j+) = g'(y_j-),\ y_j \in Y, j = 1, \ldots, N\} \end{gathered} \tag{3.6}$$

and that

$$\dot{H}'^{*}_Y \phi(k) = k^2 \phi(k), \qquad \phi(k) \in \mathscr{D}(\dot{H}'^{*}_Y), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{3.7}$$

has the solutions

$$\phi_j(k, x) = \begin{cases} e^{ik(x - y_j)}, & x > y_j, \\ -e^{ik(y_j - x)}, & x < y_j, \end{cases} \qquad \operatorname{Im} k > 0, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{3.8}$$

As a consequence all self-adjoint extensions of $\dot{H}'_Y$ are given by an N^2-parameter family of self-adjoint operators. Similar to Ch. II.2 we restrict ourselves to separated boundary conditions at each point $y_j, j = 1, \ldots, N$. Hence we introduce the following N-parameter family of closed extensions of $\dot{H}'_Y$:

$$\begin{gathered} \Xi_{\beta, Y} = -\frac{d^2}{dx^2}, \\ \mathscr{D}(\Xi_{\beta, Y}) = \{g \in H^{2,2}(\mathbb{R} - Y) | g'(y_j+) = g'(y_j-), \\ g(y_j+) - g(y_j-) = \beta_j g'_j(y_j), j = 1, \ldots, N\}, \\ \beta = (\beta_1, \ldots, \beta_N), \quad -\infty < \beta_j \leq \infty, \quad j = 1, \ldots, N. \end{gathered} \tag{3.9}$$

The special case $\beta = 0$ (i.e., $\beta_j = 0, j = 1, \ldots, N$) leads to the kinetic energy Hamiltonian $-\Delta$ on $H^{2,2}(\mathbb{R})$. The case $\beta_{j_0} = \infty$ for some j_0 leads to a Neumann boundary condition at the point y_{j_0} (i.e., $g'(y_{j_0}+) = g'(y_{j_0}-) = 0$). Clearly, $\Xi_{\beta,Y}$ is symmetric by a simple integration by parts. In addition, $\Xi_{\beta,Y}$ is self-adjoint since $\dot{H}'_Y$ has deficiency indices (N, N) and the N boundary conditions in (3.9) are symmetric and linearly independent ([158], Theorem XIII.4.30). By definition $\Xi_{\beta,Y}$ describes N δ'-interactions centered at $y_j \in Y$, $j = 1, \ldots, N$.

In the following we summarize basic properties of $\Xi_{\beta,Y}$. We start with describing its resolvent.

Theorem 3.1. *Let $\beta_j \neq 0, j = 1, \ldots, N$. Then the resolvent of $\Xi_{\beta,Y}$ is given by*

$$(\Xi_{\beta,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} (\overline{\tilde{\tilde{\tilde{G}}}_k(\cdot - y_{j'})}, \cdot) \tilde{\tilde{\tilde{G}}}_k(\cdot - y_j),$$

$$k^2 \in \rho(\Xi_{\beta,Y}), \quad \operatorname{Im} k > 0, \quad -\infty < \beta_j \leq \infty, \quad \beta_j \neq 0, \quad y_j \in Y, \quad j = 1, \ldots, N, \tag{3.10}$$

where

$$\tilde{\Gamma}_{\beta,Y}(k) = [-(\beta_j k^2)^{-1}\delta_{jj'} + G_k(y_j - y_{j'})]_{j,j'=1}^N \tag{3.11}$$

and

$$\tilde{\tilde{G}}_k(x - y) = (i/2k)\begin{cases} e^{ik(x-y)}, & x > y, \\ -e^{ik(y-x)}, & x < y, \end{cases} \qquad G_k(x - y) = (i/2k)e^{ik|x-y|},$$

$$\operatorname{Im} k > 0. \tag{3.12}$$

PROOF. One can follow the analogous proof of Theorem 2.1.1 step by step. ∎

Clearly, the above characterization of $\Xi_{\beta,Y}$ extends to the case where some of the β_j equal zero. For example, if $\beta_{j_0} = 0$ then one simply omits the j_0th line and j_0th row in the definition of $\tilde{\Gamma}_{\beta,Y}(k)$.

Additional domain properties and locality of $\Xi_{\beta,Y}$ are discussed in

Theorem 3.2. *Let* $-\infty < \beta_j \le \infty$, $\beta_j \ne 0$, $y_j \in Y$, $j = 1, \ldots, N$. *Then the domain* $\mathscr{D}(\Xi_{\beta,Y})$ *consists of all elements* ψ *of the type*

$$\psi(x) = \phi_k(x) + (i/k) \sum_{j,j'=1}^N [\tilde{\Gamma}_{\beta,Y}(k)]_{jj'}^{-1} \phi_k'(y_{j'}) \tilde{\tilde{G}}_k(x - y_j), \tag{3.13}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ *and* $k^2 \in \rho(\Xi_{\beta,Y})$, $\operatorname{Im} k > 0$. *The decomposition* (3.13) *is unique and with* $\psi \in \mathscr{D}(\Xi_{\beta,Y})$ *of this form we obtain*

$$(\Xi_{\beta,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{3.14}$$

Next let $\psi \in \mathscr{D}(\Xi_{\beta,Y})$ *and suppose that* $\psi = 0$ *in an open set* $U \subseteq \mathbb{R}$. *Then* $\Xi_{\beta,Y}\psi = 0$ *in* U.

PROOF. Identical to that of Theorem 2.1.2 since

$$(\tilde{\tilde{G}}_k(\cdot - y), (-\Delta - k^2)\phi) = (i/k)\phi'(y), \qquad \phi \in H^{2,2}(\mathbb{R}), \quad y \in \mathbb{R}. \tag{3.15}$$

∎

Spectral properties of $\Xi_{\beta,Y}$ are given in

Theorem 3.3. *Let* $\beta_j \ne 0$, $y_j \in Y$, $j = 1, \ldots, N$. *Assume that at most one* $\beta_{j_0} = \infty$. *Then* $\Xi_{\beta,Y}$ *has at most* N *eigenvalues which are all negative and simple. If* $\beta_j = \infty$ *for at least two different values* $j \in \{1, \ldots, N\}$, *then* $\Xi_{\beta,Y}$ *has at most* N *negative eigenvalues (counting multiplicity) and infinitely many eigenvalues embedded in* $[0, \infty)$ *accumulating at* ∞. *In particular,*

$$k^2 \in \sigma_p(\Xi_{\beta,Y}) \cap (-\infty, 0) \quad \textit{iff} \quad \det[\tilde{\Gamma}_{\beta,Y}(k)] = 0, \qquad \operatorname{Im} k > 0, \tag{3.16}$$

and the multiplicity of the eigenvalue $k^2 < 0$ *equals the multiplicity of the eigenvalue zero of the matrix* $\tilde{\Gamma}_{\beta,Y}(k)$. *Moreover, if* $E_0 = k_0^2 < 0$ *is an eigenvalue of* $\Xi_{\beta,Y}$, *the corresponding eigenfunctions are of the form*

$$\psi_0(x) = \sum_{j=1}^N \tilde{c}_j \tilde{\tilde{G}}_{k_0}(x - y_j), \qquad \operatorname{Im} k_0 > 0, \tag{3.17}$$

where $(\tilde{c}_1, \ldots, \tilde{c}_N)$ *are eigenvectors of the matrix* $\tilde{\Gamma}_{\beta,Y}(k_0)$ *to the eigenvalue zero.*

The remaining part of the spectrum is absolutely continuous and covers the nonnegative real line

$$\sigma_{\text{ess}}(\Xi_{\beta,Y}) = \sigma_{\text{ac}}(\Xi_{\beta,Y}) = [0, \infty), \qquad \sigma_{\text{sc}}(\Xi_{\beta,Y}) = \varnothing,$$
$$-\infty < \beta_j \leq \infty, \quad j = 1, \ldots, N. \tag{3.18}$$

PROOF. Since $\dot{H}'_Y \geq 0$ and $\dot{H}'_Y$ has deficiency indices (N, N), $\Xi_{\beta,Y}$ has at most N negative eigenvalues counting multiplicity ([494], p. 246). Moreover, (3.16) and (3.17) then follow as in Theorem 1.1.4 and all assertions in (3.18) follow as in Theorem I.3.1.4. It remains to prove the statements concerning the point spectrum. We closely follow the analogous treatment in Theorem 2.1.3. Without loss of generality assume

$$y_1 < y_2 < \cdots < y_N. \tag{3.19}$$

If all $|\beta_j| < \infty, j = 1, \ldots, N$, we define

$$\psi_k(x) = \begin{cases} a_1 e^{ikx} + b_1 e^{-ikx}, & x < y_1, \\ a_{m+1} e^{ikx} + b_{m+1} e^{-ikx}, & y_m < x < y_{m+1}, \quad 1 \leq m \leq N-1, \\ a_{N+1} e^{ikx} + b_{N+1} e^{-ikx}, & x > y_N; \quad \operatorname{Im} k > 0, \quad k \neq 0, \end{cases} \tag{3.20}$$

where a_{m+1} and b_{m+1} are unique (nontrivial) solutions of

$$a_{m+1} e^{iky_m} - b_{m+1} e^{-iky_m} = a_m e^{iky_m} - b_m e^{-iky_m},$$
$$a_{m+1} e^{iky_m}[1 - ik\beta_m] + b_{m+1} e^{-iky_m}[1 + ik\beta_m] = a_m e^{iky_m} + b_m e^{-iky_m}, \quad m = 1, \ldots, N,$$
$$a_1 = a, \qquad b_1 = b, \qquad a, b \in \mathbb{R}. \tag{3.21}$$

Then $\psi_k(x)$ obeys

$$\psi'_k(y_j+) = \psi'_k(y_j-), \qquad \psi_k(y_j+) - \psi_k(y_j-) = \beta_j \psi'_k(y_j), \qquad j = 1, \ldots, N. \tag{3.22}$$

In addition, by the uniqueness of the coefficients a_{m+1}, b_{m+1}, $1 \leq m \leq N$, ψ_k is the unique solution (up to multiplicative constants) of

$$-\psi''_k(x) = k^2 \psi_k(x), \qquad x \in \mathbb{R} - Y, \tag{3.23}$$

obeying $\psi_k \in H^{2,2}_{\text{loc}}(\mathbb{R} - Y)$ and the boundary conditions (3.22). If $k^2 > 0$, then $\psi_k \in L^2(\mathbb{R})$ iff $a = b = 0$ implying $\psi_k = 0$. Since the same argument applies for $k = 0$ (replace $e^{\pm ikx}$ by 1, x in (3.20)) we obtain $\sigma_p(\Xi_{\beta,Y}) \subset (-\infty, 0)$ in this case. For $k^2 < 0$ we get $a = 0$ and the above-mentioned uniqueness proves the simplicity of the eigenvalue. (In fact, $k^2 < 0$ corresponds to an eigenvalue of $\Xi_{\beta,Y}$ iff $b_{N+1} = 0$.)

Next consider the case where precisely one of the β_j, say $\beta_{j_0} = \infty$ and $N \geq 2$ (for $N = 1$, cf. Theorem I.4.3). Then the boundary condition at y_{j_0} reduces to $g'(y_{j_0}\pm) = 0$ (with no condition on $g(y_{j_0}\pm)$), i.e., it becomes a Neumann boundary condition and hence decouples $\mathbb{R}$ into $(-\infty, y_{j_0})$ and (y_{j_0}, ∞). It suffices to consider (y_{j_0}, ∞). If necessary we renumber $y_{j_0} < y_{j_0+1} < \cdots < y_N$ to get $\tilde{y}_1 < \tilde{y}_2 < \cdots < \tilde{y}_M$ for some $M \leq N$. Then we introduce

$$\psi_k(x) = \begin{cases} \tilde{a} \cos[k(x - \tilde{y}_1)], & \tilde{y}_1 < x < \tilde{y}_2, \\ \tilde{a}_{m+1} e^{ikx} + \tilde{b}_{m+1} e^{-ikx}, & \tilde{y}_m < x < \tilde{y}_{m+1}, \quad 2 \leq m \leq M-1, \\ \tilde{a}_{M+1} e^{ikx} + \tilde{b}_{M+1} e^{-ikx}, & x > \tilde{y}_M; \quad \operatorname{Im} k \geq 0, \quad k \neq 0, \end{cases} \tag{3.24}$$

where now $\tilde{a}_{m+1}$ and $\tilde{b}_{m+1}$ are unique (nontrivial) solutions of

$$\tilde{a}_{m+1}e^{ik\tilde{y}_m} - \tilde{b}_{m+1}e^{-ik\tilde{y}_m} = \tilde{a}_m e^{ik\tilde{y}_m} - \tilde{b}_m e^{-ik\tilde{y}_m},$$
$$\tilde{a}_{m+1}e^{ik\tilde{y}_m}[1 - ik\beta_m] + \tilde{b}_{m+1}e^{-ik\tilde{y}_m}[1 + ik\beta_m] = \tilde{a}_m e^{ik\tilde{y}_m} + \tilde{b}_m e^{-ik\tilde{y}_m},$$
$$3 \le m \le M, \quad (3.25)$$
$$\tilde{a}_3 e^{ik\tilde{y}_2} - \tilde{b}_3 e^{-ik\tilde{y}_2} = i\tilde{a}\sin[k(\tilde{y}_2 - \tilde{y}_1)],$$
$$\tilde{a}_3 e^{ik\tilde{y}_2}[1 - ik\beta_2] + \tilde{b}_3 e^{-ik\tilde{y}_2}[1 + ik\beta_2] = \tilde{a}\cos[k(\tilde{y}_2 - \tilde{y}_1)].$$

Then ψ_k fulfills $\psi_k \in AC_{\text{loc}}((\tilde{y}_1, \infty) - \{\tilde{y}_2, \ldots, \tilde{y}_M\})$, $\psi_k' \in AC_{\text{loc}}((\tilde{y}_1, \infty))$ and

$$\psi_k'(\tilde{y}_1+) = 0,$$
$$\psi_k'(\tilde{y}_j+) = \psi_k'(\tilde{y}_j-), \qquad \psi_k(\tilde{y}_j+) - \psi_k(\tilde{y}_j-) = \beta_j\psi_k'(\tilde{y}_j), \qquad j = 2, \ldots, M. \quad (3.26)$$

Hence ψ_k uniquely solves (up to multiplicative constants)

$$-\psi_k''(x) = k^2\psi_k(x), \qquad \tilde{y}_1 < x < \infty, \quad x \neq \tilde{y}_2, \ldots, \tilde{y}_M \quad (3.27)$$

and the boundary conditions (3.26). If $k^2 > 0$, then $\psi_k \in L^2((\tilde{y}_1, \infty))$ implies $\tilde{a}_{M+1} = \tilde{b}_{M+1} = 0$ and hence $\psi_k = 0$. The same argument works for $k = 0$. Since the analogous construction applies for the interval $(-\infty, \tilde{y}_{j_0})$, and $\Xi_{\beta,Y}$ is the direct sum of the corresponding operators in $L^2((-\infty, y_{j_0}))$ and $L^2((y_{j_0}, \infty))$ we obtain again $\sigma_p(\Xi_{\beta,Y}) \subset (-\infty, 0)$. Simplicity of negative eigenvalues then follows by the uniqueness of ψ_k.

That $\Xi_{\beta,Y}$ has infinitely many eigenvalues embedded in $[0, \infty)$ accumulating at ∞ if $\beta_j = \infty$, for at least two different values of $j \in \{1, \ldots, N\}$, follows exactly by the arguments in the proof of Theorem 2.1.3. ∎

As in the one-center case the pole structure in (3.10) determines bound states as well as resonances of $\Xi_{\beta,Y}$. In particular, any solution k_1 of $\det[\tilde{\Gamma}_{\beta,Y}(k_1)] = 0$ with $\operatorname{Im} k_1 < 0$ defines a resonance of $\Xi_{\beta,Y}$ whose multiplicity by definition coincides with the multiplicity of the zero of $\det[\tilde{\Gamma}_{\beta,Y}(k)]$ at $k = k_1$. At $k = 0$, $\tilde{\Gamma}_{\beta,Y}(0)$ does not exist and hence one is forced to consider $[\tilde{\Gamma}_{\beta,Y}(k)]^{-1}$ as $k \to 0$.

It remains to discuss stationary scattering theory for the pair $(\Xi_{\beta,Y}, -\Delta)$. The generalized eigenfunctions of $\Xi_{\beta,Y}$ are given by

$$\Psi_{\beta,Y}(k, \sigma, x) = e^{ik\sigma x} - \sum_{j,j'=1}^{N} \sigma[\tilde{\Gamma}_{\beta,Y}(k)]_{jj'}^{-1} e^{ik\sigma y_{j'}} \tilde{\tilde{G}}_k(x - y_j),$$
$$\sigma = \pm 1, \quad -\infty < \beta_j \le \infty, \quad \beta_j \neq 0, \quad y_j \in Y, \quad j = 1, \ldots, N, \quad x \in \mathbb{R}. \quad (3.28)$$

By inspection they fulfill

$$\Psi_{\beta,Y}'(k, \sigma, y_j+) = \Psi_{\beta,Y}'(k, \sigma, y_j-),$$
$$\Psi_{\beta,Y}(k, \sigma, y_j+) - \Psi_{\beta,Y}(k, \sigma, y_j-) = \beta_j\Psi_{\beta,Y}'(k, \sigma, y_j),$$
$$-\Psi_{\beta,Y}''(k, \sigma, x) = k^2\Psi_{\beta,Y}(k, \sigma, x), \qquad x \in \mathbb{R} - Y,$$
$$\lim_{\varepsilon \downarrow 0} \lim_{x' \to \mp\infty} (2k/i)e^{\pm i(k+i\varepsilon)x'}[\Xi_{\beta,Y} - (k + i\varepsilon)^2]^{-1}(x, x') = \Psi_{\beta,Y}(k, \pm 1, x),$$
$$x \in \mathbb{R}; \quad k > 0. \quad (3.29)$$

The corresponding *transmission* and *reflection coefficients* from the left and right then read

$$\begin{aligned}
\mathscr{T}^{l}_{\beta,Y}(k) &= \lim_{x\to+\infty} e^{-ikx}\Psi_{\beta,Y}(k, +1, x)\\
&= 1 + (2ik)^{-1} \sum_{j,j'=1}^{N} e^{-iky_j}[\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} e^{iky_{j'}},\\
\mathscr{T}^{r}_{\beta,Y}(k) &= \lim_{x\to-\infty} e^{ikx}\Psi_{\beta,Y}(k, -1, x)\\
&= 1 + (2ik)^{-1} \sum_{j,j'=1}^{N} e^{iky_j}[\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} e^{-iky_{j'}} = \mathscr{T}^{l}_{\beta,Y}(k),\\
\mathscr{R}^{l}_{\beta,Y}(k) &= \lim_{x\to-\infty} e^{ikx}[\Psi_{\beta,Y}(k, +1, x) - e^{ikx}] \qquad (3.30)\\
&= -(2ik)^{-1} \sum_{j,j'=1}^{N} e^{iky_j}[\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} e^{iky_{j'}},\\
\mathscr{R}^{r}_{\beta,Y}(k) &= \lim_{x\to+\infty} e^{-ikx}[\Psi_{\beta,Y}(k, -1, x) - e^{-ikx}]\\
&= -(2ik)^{-1} \sum_{j,j'=1}^{N} e^{-iky_j}[\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} e^{-iky_{j'}};\\
&\qquad k > 0, \quad -\infty < \beta_j \le \infty, \quad \beta_j \ne 0, \quad y_j \in Y, \quad j = 1, \ldots, N.
\end{aligned}$$

The unitary on-shell scattering operator $\mathscr{S}_{\beta,Y}(k)$ in $\mathbb{C}^2$ is then defined as

$$\mathscr{S}_{\beta,Y}(k) = \begin{bmatrix} \mathscr{T}^{l}_{\beta,Y}(k) & \mathscr{R}^{r}_{\beta,Y}(k) \\ \mathscr{R}^{l}_{\beta,Y}(k) & \mathscr{T}^{r}_{\beta,Y}(k) \end{bmatrix},$$

$$k > 0, \quad -\infty < \beta_j \le \infty, \quad \beta_j \ne 0, \quad y_j \in Y, \quad j = 1, \ldots, N, \qquad (3.31)$$

and obviously $\mathscr{S}_{\beta,Y}(k)$ has a meromorphic continuation in k to all of $\mathbb{C}$ such that poles of $\mathscr{S}_{\beta,Y}(k)$ in $\mathbb{C} - \{0\}$ coincide with bound states or resonances of $\Xi_{\beta,Y}$.

We end up with a few remarks concerning the definition of a mixture of δ- and δ'-interactions in the N-center case ($N \ge 2$). The self-adjoint extension $H_{\alpha,\beta,Y}$ of $\dot{H}_Y$

$$\begin{aligned}
H_{\alpha,\beta,Y} &= -\frac{d^2}{dx^2},\\
\mathscr{D}(H_{\alpha,\beta,Y}) &= \{g \in H^{2,2}(\mathbb{R} - Y) | g(y_j+) = g(y_j-), g'(y_j+) - g'(y_j-) = \alpha_j g(y_j),\\
&\qquad -\infty < \alpha_j \le \infty, j \in N_\alpha; g'(y_l+) = g'(y_l-),\\
&\qquad g(y_l+) - g(y_l-) = \beta_l g'(y_l), -\infty < \beta_l \le \infty, l \in N_\beta\}, \qquad (3.32)
\end{aligned}$$

where $N_\alpha \cup N_\beta = \{1, \ldots, N\}, N_\alpha \cap N_\beta = \varnothing, N \ge 2$, represents δ-interactions at the points $y_j, j \in N_\alpha$, and δ'-interactions at y_l, $l \in N_\beta$. Clearly, one can analyze $H_{\alpha,\beta,Y}$ along the lines of Ch. 2 and the present one.

Notes

The results of this chapter are taken from [205].

CHAPTER II.4

Finitely Many Point Interactions in Two Dimensions

Finally, we generalize the content of Ch. I.5 to finitely many point interactions in two dimensions.

Let $N \in \mathbb{N}$ and introduce the set $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}^2$. We consider in $L^2(\mathbb{R}^2)$ the nonnegative operator

$$-\Delta|_{C_0^\infty(\mathbb{R}^2 - Y)} \tag{4.1}$$

with $\dot{H}_Y$ its closure in $L^2(\mathbb{R}^2)$ (i.e., $\mathscr{D}(\dot{H}_Y) = H_0^{2,2}(\mathbb{R}^2 - Y)$). The adjoint operator of $\dot{H}_Y$ then reads

$$\dot{H}_Y^* = -\Delta, \qquad \mathscr{D}(\dot{H}_Y^*) = \{g \in H_{\mathrm{loc}}^{2,2}(\mathbb{R}^2 - Y) \cap L^2(\mathbb{R}^2) | \Delta g \in L^2(\mathbb{R}^2)\}. \tag{4.2}$$

Since the equation

$$\dot{H}_Y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_Y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{4.3}$$

has the solutions

$$\psi_j(k, x) = (i/4) H_0^{(1)}(k|x - y_j|), \qquad x \in \mathbb{R}^2 - \{y_j\},$$
$$\operatorname{Im} k > 0, \quad y_j \in Y, \quad j = 1, \ldots, N \tag{4.4}$$

(we recall that $H_0^{(1)}(\cdot)$ denotes the Hankel function of first kind and order zero [1]), $\dot{H}_Y$ has deficiency indices (N, N). Thus all self-adjoint extensions of $\dot{H}_Y$ are given by an N^2-parameter family of self-adjoint operators. In order to find the two-dimensional analog of our N-center δ-interactions in one and three dimensions we proceed as follows: In general, self-adjoint extensions $H_{U,Y}$ of $\dot{H}_Y$ are given by

$$\mathscr{D}(H_{U,Y}) = \left\{ g + \sum_{j=1}^{N} c_j \left[\psi_{j+} + \sum_{j'=1}^{N} U_{jj'} \psi_{j'-} \right] \middle| g \in \mathscr{D}(\dot{H}_Y),\ c_j \in \mathbb{C},\ j = 1, \ldots, N \right\},$$

$$H_{U,Y}\left\{ g + \sum_{j=1}^{N} c_j \left[\psi_{j+} + \sum_{j'=1}^{N} U_{jj'} \psi_{j'-} \right] \right\}$$

$$= \dot{H}_Y g + i \sum_{j=1}^{N} c_j \left[\psi_{j+} - \sum_{j,j'=1}^{N} U_{jj'} \psi_{j'-} \right], \tag{4.5}$$

where $U_{jj'}, j, j' = 1, \ldots, N$, denotes a unitary matrix in $\mathbb{C}^N$ and

$$\psi_{j\pm}(x) = \psi_j(\sqrt{\pm i}, x) = (i/4)H_0^{(1)}(\sqrt{\pm i}\,|x - y_j|),$$
$$x \in \mathbb{R}^2 - \{y_j\}, \quad \operatorname{Im} \sqrt{\pm i} > 0, \tag{4.6}$$

provide a basis for $\operatorname{Ker}[\dot{H}_Y^* \mp i]$, respectively. Obviously, the special case $U = -1$ leads to the kinetic energy operator in $L^2(\mathbb{R}^2)$

$$H_{-1,Y} = -\Delta, \qquad \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2) \tag{4.7}$$

(since $\psi_{j+} - \psi_{j-} \in H^{2,2}(\mathbb{R}^2)$, $j = 1, \ldots, N$). Applying now Krein's formula (cf. Theorem A.3) we get

$$(H_{U,Y} - k^2)^{-1} = (-\Delta - k^2)^{-1} + \sum_{j,j'=1}^{N} \lambda(k)_{jj'}(\psi_{j'}(-\bar{k}), \cdot)\psi_j(k),$$
$$k^2 \in \rho(H_{U,Y}), \quad U \neq -1, \tag{4.8}$$

where

$$\psi_j(k, x) = \psi_j(k', x) + (k^2 - k'^2)((-\Delta - k^2)^{-1}\psi_j(k'))(x)$$
$$= (i/4)H_0^{(1)}(k|x - y_j|), \qquad \operatorname{Im} k > 0, \quad \operatorname{Im} k' > 0, \tag{4.9}$$

and

$$[\lambda(k)]_{jj'}^{-1} - [\lambda(k')]_{jj'}^{-1}$$
$$= -(k^2 - k'^2)(\psi_{j'}(-\bar{k}), \psi_j(k'))$$
$$= \psi_j(k', y_{j'}) - \psi_{j'}(k, y_j)$$
$$= \begin{cases} (2\pi)^{-1} \ln(k/k'), & j = j', \\ (i/4)[H_0^{(1)}(k'|y_j - y_{j'}|) - H_0^{(1)}(k|y_j - y_{j'}|)], & j \neq j', \end{cases}$$
$$k^2, k'^2 \in \rho(H_{U,Y}), \quad \operatorname{Im} k > 0, \quad \operatorname{Im} k' > 0. \tag{4.10}$$

The second equalities in (4.9) and (4.10) follow from the first resolvent formula

$$(k^2 - k'^2)G_k G_{k'} = G_k - G_{k'}, \qquad \operatorname{Im} k > 0, \quad \operatorname{Im} k' > 0, \tag{4.11}$$

where

$$G_k = (-\Delta - k^2)^{-1}, \qquad \operatorname{Im} k > 0, \tag{4.12}$$

denotes the free resolvent with integral kernel

$$G_k(x - x') = (i/4)H_0^{(1)}(k|x - x'|), \qquad \operatorname{Im} k > 0, \quad x, x' \in \mathbb{R}^2, \quad x \neq x'. \tag{4.13}$$

From

$$(H_{U,Y} - k^2)\left[\psi_{j+} + \sum_{j'=1}^{N} U_{jj'}\psi_{j'-}\right] = (i - k^2)\psi_{j+} - (i + k^2)\sum_{j'=1}^{N} U_{jj'}\psi_{j'-},$$
$$j = 1, \ldots, N, \tag{4.14}$$

we infer

$$\begin{aligned}(H_{U,Y} + i)^{-1}\psi_{j+} &= (2i)^{-1}\left[\psi_{j+} + \sum_{j'=1}^{N} U_{jj'}\psi_{j'-}\right]\\ &= (-\Delta + i)^{-1}\psi_{j+} + \sum_{j',j''=1}^{N} \lambda(\sqrt{-i})_{j'j''}(\psi_{j''+}, \psi_{j+})\psi_{j'-}\\ &= (2i)^{-1}(\psi_{j+} - \psi_{j-}) + \sum_{j',j''=1}^{N} \lambda(\sqrt{-i})_{j'j''}(\psi_{j''+}, \psi_{j+})\psi_{j'-},\end{aligned}$$
$$j = 1, \ldots, N, \tag{4.15}$$

implying

$$U_{jj'} + \delta_{jj'} = 2i \sum_{j''=1}^{N} (\psi_{j+}, \psi_{j''+})^{\mathrm{T}}[\lambda(\sqrt{-i})]^{\mathrm{T}}_{j''j'}, \qquad j, j' = 1, \ldots, N, \tag{4.16}$$

since $\psi_{j'-}$, $j' = 1, \ldots, N$, are linearly independent. (Here $M^{\mathrm{T}}_{jj'} = M_{j'j}$, $j, j' = 1, \ldots, N$, denotes the transposed matrix in $\mathbb{C}^N$.) Clearly, relation (4.16) is valid in general since in deriving it we only used (4.5) and Krein's formula for the pair $(H_{U,Y}, H_{-1,Y})$. Now we utilize the symmetry of $(\psi_{j+}, \psi_{j''+})$ with respect to j and j'' (i.e., $(\psi_{j+}, \psi_{j''+}) = (\psi_{j''+}, \psi_{j+})$, $j, j'' = 1, \ldots, N$) to get

$$\begin{aligned}U_{jj'} &= -\delta_{jj'} + \sum_{j''=1}^{N} \{[\lambda(\sqrt{-i})^{-1}]^{\mathrm{T}}_{jj''} - [\lambda(\sqrt{i})^{-1}]^{\mathrm{T}}_{jj''}\}[\lambda(\sqrt{-i})]^{\mathrm{T}}_{j''j'}\\ &= -\sum_{j''=1}^{N} [\lambda(\sqrt{i})^{\mathrm{T}}]^{-1}_{jj''}[\lambda(\sqrt{-i})]^{\mathrm{T}}_{j''j'},\end{aligned} \tag{4.17}$$

or equivalently,

$$U = -[\lambda(\sqrt{i})^{\mathrm{T}}]^{-1}\lambda(\sqrt{-i})^{\mathrm{T}}. \tag{4.18}$$

Since Krein's formula (4.8) implies

$$\lambda(k)^* = \lambda(-\bar{k}), \qquad k^2 \in \rho(H_{U,Y}), \qquad \operatorname{Im} k > 0, \tag{4.19}$$

unitarity of U is equivalent to the fact that $\lambda(\sqrt{i})$ (resp. $\lambda(\sqrt{-i})$) is normal. In analogy to one and three dimensions we now define (cf. also the discussion in the Notes)

$$[\lambda(k)]_{jj'}^{-1} = [\Gamma_{\alpha,Y}(k)]_{jj'}$$
$$= (2\pi)^{-1}[2\pi\alpha_j - \Psi(1) + \ln(k/2i)]\delta_{jj'} - \tilde{G}_k(|y_j - y_{j'}|),$$
$$\alpha_j \in \mathbb{R}, \quad j, j' = 1, \ldots, N, \tag{4.20}$$

where

$$\tilde{G}_k(x) = \begin{cases} G_k(x), & x \neq 0, \\ 0, & x = 0, \end{cases} \qquad \operatorname{Im} k > 0, \tag{4.21}$$

and $\Psi(\cdot)$ denotes the digamma function [1]. (Actually it would have been sufficient to define $\lambda(\sqrt{i})^{-1}$ since then $\lambda(k)^{-1}$ follows from (4.10).) The N-center point interaction Hamiltonian $-\Delta_{\alpha,Y}$ in two dimensions is thus defined by

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G_k(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N. \tag{4.22}$$

As usual, we may extend the above definition to the case where some of the α_j equal ∞. For example, if $\alpha_{j_0} = \infty$ one simply deletes the j_0th line and j_0th row in the definition of the matrix $\Gamma_{\alpha,Y}(k)$.

Next we describe further domain properties of $-\Delta_{\alpha,Y}$ and point out its locality:

Theorem 4.1. *Let $\alpha_j \in \mathbb{R}$, $y_j \in Y$, $j = 1, \ldots, N$. Then the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}\phi_k(y_{j'})G_k(x - y_j), \tag{4.23}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2)$ and $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$. The decomposition (4.23) *is unique and with $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ of this form we get*

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{4.24}$$

Next let $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ and assume $\psi = 0$ in an open set $U \subseteq \mathbb{R}^2$. Then $-\Delta_{\alpha,Y}\psi = 0$ in U.

Proof. Identical to that of Theorem 1.1.3. ∎

Spectral properties of $-\Delta_{\alpha,Y}$ are summarized in

Theorem 4.2. *Let $\alpha_j \in \mathbb{R}$, $y_j \in Y$, $j = 1, \ldots, N$. Then the essential spectrum of $-\Delta_{\alpha,Y}$ is purely absolutely continuous and equals*

$$\sigma_{\text{ess}}(-\Delta_{\alpha,Y}) = \sigma_{\text{ac}}(-\Delta_{\alpha,Y}) = [0, \infty), \qquad \sigma_{\text{sc}}(-\Delta_{\alpha,Y}) = \varnothing. \tag{4.25}$$

In addition,

$$\sigma_p(-\Delta_{\alpha,Y}) \subset (-\infty, 0) \tag{4.26}$$

and $-\Delta_{\alpha,Y}$ *has at least one and at most* N *(negative) eigenvalues counting multiplicity. In particular,*

$$k^2 \in \sigma_p(-\Delta_{\alpha,Y}) \quad \textit{iff} \quad \det[\Gamma_{\alpha,Y}(k)] = 0, \qquad \operatorname{Im} k > 0, \tag{4.27}$$

and the multiplicity of the eigenvalue k^2 *equals the multiplicity of the eigenvalue zero of the matrix* $\Gamma_{\alpha,Y}(k)$. *If* $E_0 = k_0^2$ *is an eigenvalue of* $-\Delta_{\alpha,Y}$, *the corresponding eigenfunctions are of the form*

$$\psi_0(x) = \sum_{j=1}^{N} c_j G_{k_0}(x - y_j), \qquad \operatorname{Im} k_0 > 0, \tag{4.28}$$

where $(c_1, \ldots, c_N)$ *are eigenvectors of the matrix* $\Gamma_{\alpha,Y}(k_0)$ *to the eigenvalue zero. The ground state of* $-\Delta_{\alpha,Y}$ *is nondegenerate and the corresponding eigenfunction can be chosen to be strictly positive (i.e., the associated eigenvector* $(c_1, \ldots, c_N)$ *fulfills* $c_j > 0, j = 1, \ldots, N$).

PROOF. That $-\Delta_{\alpha,Y}$ has at most N negative eigenvalues follows from the fact that $\dot{H}_Y \geq 0$ and $\operatorname{def}(\dot{H}_Y) = (N, N)$ ([494], p. 246). To prove the existence of a ground state of $-\Delta_{\alpha,Y}$ for all $\alpha_j \in \mathbb{R}, j = 1, \ldots, N$, we observe that

$$\Gamma_{\alpha,Y}(i\kappa) \underset{\kappa \to \infty}{=} (2\pi)^{-1} \ln(\kappa/2) 1 + O((\ln \kappa)^{-1}) \tag{4.29}$$

and

$$\Gamma_{\alpha,Y}(i\kappa) \underset{\kappa \downarrow 0}{=} (2\pi)^{-1} N \ln(\kappa/2) P + O((\ln \kappa)^{-1}), \tag{4.30}$$

where P is a self-adjoint projection in $\mathbb{C}^N$

$$P = [\delta_{jj'} N^{-1}]_{j,j'=1}^{N} \tag{4.31}$$

with simple eigenvalue 1 and eigenvector $(1, \ldots, 1)$. Expansions (4.29) and (4.30) show that all eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$ tend to $+\infty$ like $(2\pi)^{-1} \ln(\kappa/2)$ as $\kappa \to \infty$ and that $\Gamma_{\alpha,Y}(i\kappa)$ has a simple eigenvalue converging to $-\infty$ like $(2\pi)^{-1} N \ln(\kappa/2)$ as $\kappa \downarrow 0$. By the monotone increase of all eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$ with respect to $\kappa > 0$ (cf. Appendix F) we obtain at least one $\kappa_0 > 0$ such that $\Gamma_{\alpha,Y}(i\kappa_0)$ has the eigenvalue zero. The rest of the proof is analogous to that of Theorem 1.1.4. ∎

As in all cases discussed before, the pole structure in (4.22) determines bound states as well as resonances of $-\Delta_{\alpha,Y}$. Similarly to the one-center case, the discussion of resonances is more involved than in one or three dimensions since $(-\Delta_{\alpha,Y} - k^2)^{-1}(x, x')$, $x \neq x'$, has a meromorphic continuation to the entire logarithmic Riemann surface.

Finally, we turn to stationary scattering theory associated with the pair $(-\Delta_{\alpha,Y}, -\Delta)$. Let

$$\Psi_{\alpha,Y}(k\omega, x) = e^{ik\omega x} + (i/4) \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} e^{ik\omega y_{j'}} H_0^{(1)}(k|x - y_j|),$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k > 0, \quad \omega \in S^1, \quad \alpha_j \in \mathbb{R}, \quad x \in \mathbb{R}^2 - Y, \quad j = 1, \ldots, N, \tag{4.32}$$

then $\Psi_{\alpha,Y}(k\omega, x)$ are the scattering wave functions of $-\Delta_{\alpha,Y}$ and

$$-(\Delta\Psi_{\alpha,Y})(k\omega, x) = k^2\Psi_{\alpha,Y}(k\omega, x), \qquad x \in \mathbb{R}^2 - Y,$$

$$\lim_{\varepsilon\downarrow 0} \lim_{\substack{|x'|\to\infty \\ -|x'|^{-1}x'=\omega}} e^{i\pi/4}[8\pi(k+i\varepsilon)]^{1/2}|x'|^{1/2}e^{-i(k+i\varepsilon)|x'|}[-\Delta_{\alpha,Y} - (k+i\varepsilon)^2]^{-1}(x, x')$$

$$= \Psi_{\alpha,Y}(k\omega, x); \qquad x \in \mathbb{R}^2 - Y, \quad k > 0, \quad \omega \in S^1. \quad (4.33)$$

The *on-shell scattering amplitude* $f_{\alpha,Y}(k, \omega, \omega')$ corresponding to $-\Delta_{\alpha,Y}$ then reads

$$f_{\alpha,Y}(k, \omega, \omega') = \lim_{\substack{|x|\to\infty \\ |x|^{-1}x=\omega}} |x|^{1/2}e^{-ik|x|}[\Psi_{\alpha,Y}(k\omega', x) - e^{ik\omega' x}]$$

$$= e^{i\pi/4}(8\pi k)^{-1/2} \sum_{j,j'=1}^{N} e^{-ik\omega y_j}[\Gamma_{\alpha,Y}(k)]^{-1}_{jj'}e^{ik\omega' y_{j'}},$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \ k > 0, \ \omega, \omega' \in S^1, \ \alpha_j \in \mathbb{R}, \ y_j \in Y, \ j = 1, \ldots, N. \quad (4.34)$$

The unitary *on-shell scattering operator* $\mathscr{S}_{\alpha,Y}(k)$ in $L^2(S^1)$ is finally given by

$$\mathscr{S}_{\alpha,Y}(k) = 1 - (4\pi i)^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'}(e^{-ik(\cdot)y_{j'}}, \cdot)e^{-ik(\cdot)y_j},$$

$$\det[\Gamma_{\alpha,Y}(k)] \neq 0, \quad k > 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N. \quad (4.35)$$

Formula (4.35) shows that $\mathscr{S}_{\alpha,Y}(k)$ has a meromorphic continuation in k to the entire logarithmic Riemann surface.

Notes

The derivation of formula (4.16) has been taken from [129] where particular attention has been paid to introducing point interactions in $L^2(\mathbb{R}^n)$, $1 \leq n \leq 3$, with general boundary conditions connecting different points in Y. The rest of this chapter appeared in [19]. We emphasize that the approach used to define the two-dimensional, N-center, δ-interaction presented there works as well in one and three dimensions. To illustrate this fact it suffices to note that

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = -\alpha_j^{-1}\delta_{jj'} - G_k(y_j - y_{j'}) = -[\alpha_j^{-1} + (i/2k)]\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})$$

$$= \begin{cases} -\alpha_j^{-1} + \lim_{|x|\downarrow 0} [G_0(x) - G_k(x)], & j = j', \\ -G_k(|y_j - y_{j'}|), & j \neq j', \quad j, j' = 1, \ldots, N, \end{cases}$$

in one dimension (where $G_0(x) = -|x|/2$, $x \in \mathbb{R}$),

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = [\alpha_j - (2\pi)^{-1}\Psi(1) + (2\pi)^{-1}\ln(k/2i)]\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})$$

$$= \begin{cases} \alpha_j + \lim_{|x|\downarrow 0} [G_0(x) - G_k(x)], & j = j', \\ -G_k(|y_j - y_{j'}|), & j \neq j', \quad j, j' = 1, \ldots, N, \end{cases}$$

in two dimensions (where $G_0(x) = -(2\pi)^{-1} \ln|x|$, $x \in \mathbb{R}^2 - \{0\}$) and

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = [\alpha_j - (ik/4\pi)]\delta_{jj'} - \tilde{G}_k(|y_j - y_{j'}|)$$

$$= \begin{cases} \alpha_j + \lim\limits_{|x|\downarrow 0} [G_0(x) - G_k(x)], & j = j', \\ -G_k(|y_j - y_{j'}|), & j \neq j', \quad j, j' = 1, \ldots, N, \end{cases}$$

in three dimensions (where $G_0(x) = (4\pi|x|)^{-1}$, $x \in \mathbb{R}^3 - \{0\}$) and

$$\tilde{G}_k(x) = \begin{cases} G_k(x), & x \neq 0 \\ 0, & x = 0. \end{cases}$$

PART III

POINT INTERACTIONS WITH INFINITELY MANY CENTERS

CHAPTER III.1

Infinitely Many Point Interactions in Three Dimensions

III.1.1 Basic Properties

Our starting point will be the point interaction Hamiltonian with a finite number of centers, and then the use of a limiting argument to show that the analogous expression is still valid when Y is infinite.

For use in later sections we will discuss the operator both in x- and p-space. Consider

$$Y = \{y_j \in \mathbb{R}^3 \mid j \in \mathbb{N}\} \subset \mathbb{R}^3 \tag{1.1.1}$$

such that

$$\inf_{\substack{j \neq j' \\ j, j' \in \mathbb{N}}} |y_j - y_{j'}| = d > 0 \tag{1.1.2}$$

and let

$$\alpha\colon Y \to \mathbb{R}. \tag{1.1.3}$$

For convenience, we shall write α_j instead of α_{y_j} to simplify the notation. Then we can define $-\Delta_{\alpha,Y}$ as a strong resolvent limit of restrictions $-\Delta_{\tilde{\alpha},\tilde{Y}}$ of $-\Delta_{\alpha,Y}$ to finite subsets $\tilde{Y}$ of Y. This is the content of the following

Theorem 1.1.1. *Let $Y = \{y_j \in \mathbb{R}^3 \mid j \in \mathbb{N}\}$ be discrete in the sense that*

$$\inf_{\substack{j \neq j' \\ j, j' \in \mathbb{N}}} |y_j - y_{j'}| = d > 0 \tag{1.1.4}$$

and let $\alpha\colon Y \to R$. *Then the strong limit in* $L^2(\mathbb{R}^3)$

$$\operatorname*{s-lim}_{\substack{\tilde{Y}\subset Y\\ |\tilde{Y}|<\infty}} (-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \tag{1.1.5}$$

over the filter of all finite subsets $\tilde{Y}$ *of* Y *exists where* $\tilde{\alpha} = \alpha|_{\tilde{Y}}$ *and* $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ *is given by* (II.1.1.33). *This limit equals the resolvent of a self-adjoint operator denoted by* $-\Delta_{\alpha,Y}$ *which has the resolvent*

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\overline{G_k(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}),\quad \operatorname{Im} k > 0,\quad y_j \in Y,\quad |y_j - y_{j'}| \geq d,\quad j \neq j',\quad j,j' \in \mathbb{N}, \tag{1.1.6}$$

where $\Gamma_{\alpha,Y}(k)$ *is the closed operator in* $l^2(Y)$ *given by*

$$\Gamma_{\alpha,Y}(k) = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right]_{j,j'\in\mathbb{N}}, \qquad \operatorname{Im} k > 0 \tag{1.1.7}$$

on $l_0(Y)$ *where*

$$l_0(Y) = \{g \in l^2(Y) | \operatorname{supp} g \textit{ finite}\}. \tag{1.1.8}$$

We have

$$[\Gamma_{\alpha,Y}(k)]^{-1} \in \mathscr{B}(l^2(Y)), \qquad k^2 \in \rho(-\Delta_{\alpha,Y}),$$
$$\operatorname{Im} k > 0 \textit{ large enough}. \tag{1.1.9}$$

If α *is bounded, then* $\Gamma_{\alpha,Y}(k)$ *is analytic in* k *for* $\operatorname{Im} k > 0$.

Let

$$-\hat{\Delta}_{\alpha,Y} = \mathscr{F}[-\Delta_{\alpha,Y}]\mathscr{F}^{-1}. \tag{1.1.10}$$

Then

$$(\hat{g}, (-\hat{\Delta}_{\alpha,Y} - k^2)^{-1}\hat{f}) = (\hat{g}, (p^2 - k^2)^{-1}\hat{f})$$
$$+ \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\hat{g}, F_{k,y_j})(F_{-\bar{k},y_{j'}}, \hat{f}),$$
$$k^2 \in \rho(-\hat{\Delta}_{\alpha,Y}),\quad \operatorname{Im} k > 0,\quad \alpha_j \in \mathbb{R},\quad y_j \in Y,$$
$$|y_j - y_{j'}| \geq d,\quad j \neq j',\quad j,j' \in \mathbb{N},\quad \hat{f}, \hat{g} \in L^2(\mathbb{R}^3), \tag{1.1.11}$$

where

$$F_{k,y_j}(p) = (2\pi)^{-3/2}\frac{e^{-ipy_j}}{p^2 - k^2}, \qquad p \in \mathbb{R}^3,\quad j \in \mathbb{N}. \tag{1.1.12}$$

PROOF. For each finite subset $\tilde{Y}$ of Y we have that $-\Delta_{\tilde{\alpha},\tilde{Y}}, \tilde{\alpha} = \alpha|_{\tilde{Y}}$ has the resolvent

$$(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{\infty} [\Gamma_{\tilde{\alpha},\tilde{Y}}(k)]_{jj'}^{-1}(\overline{G_k(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j),$$
$$k^2 \in \rho(-\Delta_{\tilde{\alpha},\tilde{Y}}),\quad \operatorname{Im} k > 0, \tag{1.1.13}$$

where the matrix inverse is an operator in $l^2(\tilde{Y})$, i.e., a $|\tilde{Y}| \times |\tilde{Y}|$-matrix. First, we observe that there exists a $k_0^2 < 0$, $\operatorname{Im} k_0 > 0$, such that the resolvent $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ exists for all $k^2 > k_0^2$ and is increasing in $\tilde{Y}$, i.e.,

$$\tilde{Y} \subseteq \bar{Y} \quad \text{implies} \quad (-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1} \leq (-\Delta_{\bar{\alpha},\bar{Y}} - k^2)^{-1}, \qquad k^2 \leq k_0^2, \quad (1.1.14)$$

for all $\tilde{Y}, \bar{Y} \subseteq Y$, $|\tilde{Y}|, |\bar{Y}| < \infty$, where k_0^2 is independent of the subsets $\tilde{Y}$ and $\bar{Y}$. This can be seen as follows: We showed in the proof of Theorem II.1.1.1 that the operator $-\Delta_{\tilde{\alpha},\tilde{Y}}$ is approximated in norm resolvent sense by the operators

$$\hat{H}_{\tilde{Y}}^{\omega} = p^2 - \sum_{\substack{j \in \mathbb{N} \\ y_j \in \tilde{Y}}} \mu_j(\omega)(\phi_{y_j}^{\omega}, \cdot)\phi_{y_j}^{\omega}, \quad \mu_j(\omega) = \left(\alpha_j + \frac{\omega}{2\pi^2}\right)^{-1}, \qquad j \in \mathbb{N}, \quad (1.1.15)$$

as $\omega \to \infty$. For $\omega > 0$ large enough, $\mu_j(\omega)$ is positive, thus making the operators $\hat{H}_{\tilde{Y}}^{\omega}$ monotone decreasing in $\tilde{Y}$. Hence the resolvents of $\hat{H}_{\tilde{Y}}^{\omega}$ are monotone increasing in $\tilde{Y}$ whenever they exist. By letting $\omega \to \infty$ we obtain the same property for the resolvents of $-\hat{\Delta}_{\tilde{\alpha},\tilde{Y}}$ and thus for the resolvents of $-\Delta_{\tilde{\alpha},\tilde{Y}}$ whenever they exist. To prove the existence of such a $k_0^2 < 0$ it is then sufficient to prove that the matrix $\Gamma_{\tilde{\alpha},\tilde{Y}}(k)$ is invertible for all subsets $\tilde{Y}$ of Y and all k with $\operatorname{Im} k > 0$ sufficiently large. To this end, consider the bounded operator $\tilde{G}_k$ on $l^2(Y)$ with kernel $\tilde{G}_k(y_j - y_{j'})$, i.e.,

$$(\tilde{G}_k g)(y_j) = \sum_{j'=1}^{\infty} \tilde{G}_k(y_j - y_{j'})g(y_{j'}), \qquad \operatorname{Im} k > 0, \quad g = \{g(y_j)\}_{j \in \mathbb{N}} \in l^2(Y). \quad (1.1.16)$$

Using Lemma C.3 we infer that in order to control the norm of $\tilde{G}_k$ it suffices to bound the quantity

$$\sup_{j \in \mathbb{N}} \sum_{j'=1}^{\infty} |\tilde{G}_k(y_j - y_{j'})| \leq \frac{1}{4\pi d} \sup_{j \in \mathbb{N}} \sum_{\substack{j'=1 \\ j' \neq j}}^{\infty} e^{-\operatorname{Im} k |y_j - y_{j'}|}. \quad (1.1.17)$$

Since there is at most one point $y_{j'} \in Y$ inside each cube of size $d/2$ centered at

$$y_j + \frac{d}{2}\mathbb{Z}^3, \quad (1.1.18)$$

we obtain that the right-hand side of (1.1.17) can be estimated by

$$\frac{1}{4\pi d} \sum_{j \in \mathbb{Z}^3 - \{0\}} e^{-\operatorname{Im} k |j| d/2} \quad (1.1.19)$$

which can be made arbitrarily small by choosing $\operatorname{Im} k > 0$ sufficiently large. Thus $\tilde{G}_k$ tends to zero in norm as $\operatorname{Im} k \to \infty$, and hence $\Gamma_{\alpha,Y}(k)$ is invertible for all k with $\operatorname{Im} k > 0$ sufficiently large and $ik \notin \{4\pi\alpha_j | j \in \mathbb{N}\}$. But then the restrictions of the matrix $\Gamma_{\alpha,Y}(k)$ to arbitrary subsets of Y are also invertible. Using

$$\|(S - z)^{-1}\| = d(z, \sigma(S))^{-1} \quad (1.1.20)$$

for self-adjoint operators S, where $d(\cdot, \cdot)$ denotes the distance, we have proved that the increasing filter of operators $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$, $\tilde{Y} \subseteq Y$, $|\tilde{Y}| < \infty$, $\tilde{\alpha} = \alpha|_{\tilde{Y}}$, is uniformly bounded, viz.

$$\|(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}\| \leq |k^2 - k_0^2|^{-1}. \quad (1.1.21)$$

From Vigier's theorem ([480], p. 51) we obtain that

$$R(k^2) = \operatorname*{s-lim}_{\substack{\tilde{Y} \subset Y \\ |\tilde{Y}| < \infty}} (-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1} \quad (1.1.22)$$

exists and equals the unique supremum of the strong closure of the filter. By the explicit characterization of the resolvent of $-\Delta_{\tilde{\alpha},\tilde{Y}}$ we see that $R(k^2)$ reads

$$(R(k^2)f)(x) = (G_k f)(x) + \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} (\overline{G_k(\cdot - y_{j'})}, f) G_k(x - y_j),$$

$$\operatorname{Re} k \neq 0, \quad \operatorname{Im} k > 0, \quad x \in \mathbb{R}^3 - Y, \quad f \in L^2(\mathbb{R}^3), \quad (1.1.23)$$

whenever the right-hand side exists and defines an element in $L^2(\mathbb{R}^3)$. The following argument implies that (1.1.23) is well defined for all $f \in L^2(\mathbb{R}^3)$. Let

$$a(f) = \{a_j(f)\}_{j \in \mathbb{N}}, \qquad a_j(f) = (\overline{G_k(\cdot - y_j)}, f), \quad j \in \mathbb{N}, \quad f \in L^2(\mathbb{R}^3). \quad (1.1.24)$$

Then

$$(g, R(k^2)f) = (g, G_k f) + \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} \overline{a_j(g)} a_{j'}(f)$$

$$= (g, G_k f) + (a(g), [\Gamma_{\alpha,Y}(k)]^{-1} a(f))_{l^2(Y)}, \qquad f, g \in L^2(\mathbb{R}^3), \quad (1.1.25)$$

provided $a(f), a(g) \in l^2(Y)$. Hence, it is sufficient to prove that $\{h(y_j)\}_{j \in \mathbb{N}} \in l^2(Y)$ for all $h \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^3)$. Assume that $h \in \mathscr{D}(-\Delta)$. Then h is continuous ([283], p. 301) and equals

$$h(x) = \int d^3x' \, G_{i\kappa}(x - x') f(x'), \qquad \kappa \in (0, \infty), \quad (1.1.26)$$

for some $f \in L^2(\mathbb{R}^3)$. It is sufficient to consider the case where $Y = \mathbb{Z}^3$ since Y is discrete. Writing

$$\mathbb{R}^3 = \bigcup_{j' \in \mathbb{Z}^3} (j' + Q), \quad (1.1.27)$$

where $Q = [0, 1)^3 \subset \mathbb{R}^3$, we see that

$$|h(x)| \leq \sum_{j' \in \mathbb{Z}^3} \int_{j'+Q} d^3x' \frac{e^{-\kappa|x-x'|}}{4\pi|x - x'|} |f(x')|$$

$$\leq \sum_{j' \in \mathbb{Z}^3} \left[\int_{j'+Q} d^3x' \frac{e^{-2\kappa|x-x'|}}{16\pi^2|x - x'|^2} \right]^{1/2} \left[\int_{j'+Q} d^3x' \, |f(x')|^2 \right]^{1/2}. \quad (1.1.28)$$

Since

$$\tilde{f} = \{f_{j'}\}_{j' \in \mathbb{Z}^3} \in l^2(\mathbb{Z}^3), \qquad f_{j'} = \left[\int_{j'+Q} d^3x' |f(x')|^2 \right]^{1/2}, \quad (1.1.29)$$

it suffices to prove that the matrix

$$M = [M_{jj'}]_{j,j' \in \mathbb{Z}^3}, \qquad M_{jj'} = \int_{j'+Q} d^3x' \frac{e^{-2\kappa|j-x'|}}{16\pi^2|j - x'|^2} \quad (1.1.30)$$

is bounded. We have

$$M_{jj'} = \int_Q d^3x' \frac{e^{-2\kappa|j-j'-x'|}}{16\pi^2|j - j' - x'|^2} \leq ce^{-2\kappa|j-j'|} \quad (1.1.31)$$

which proves (by Lemma C.3) that the Holmgren bound of M exists. ∎

We end this section with a characterization of the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ of $-\Delta_{\alpha,Y}$ and with the proof that $-\Delta_{\alpha,Y}$ is still local when Y is infinite.

Theorem 1.1.2. *Let $y_j \in Y$, $|y_j - y_{j'}| \geq d > 0$, $j \neq j'$, and let $\alpha_j \in \mathbb{R}$, $j, j' \in \mathbb{N}$. Then the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ of $-\Delta_{\alpha,Y}$ is the set of all ψ such that*

$$\psi(x) = \phi_k(x) + \sum_{j=1}^{\infty} a_j(k) G_k(x - y_j), \qquad x \in \mathbb{R}^3 - Y, \tag{1.1.32}$$

for some k with $\operatorname{Im} k > 0$, where

$$\phi_k \in \mathscr{D}(-\Delta), \qquad a_j(k) = \sum_{j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} \phi_k(y_{j'}). \tag{1.1.33}$$

Furthermore, this decomposition is unique and

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k, \tag{1.1.34}$$

and if $\psi = 0$ in an open set $U \subseteq \mathbb{R}^3$, then also $-\Delta_{\alpha,Y}\psi = 0$ in U.

PROOF. Using that $\phi \in \mathscr{D}(-\Delta)$ implies that $\{\phi(y_j)\}_{j \in \mathbb{N}} \in l^2(Y)$ (cf. the proof of Theorem 1.1.1) we infer that the proof of Theorem II.1.1.2 still applies. ∎

As in Part II, we extend our definition of $-\Delta_{\alpha,Y}$ to allow $\alpha_{y_{j_0}} = \infty$ for some $j_0 \in \mathbb{N}$ in the sense that $-\Delta_{\alpha,Y} = -\Delta_{\tilde{\alpha},\tilde{Y}}$ where $\tilde{\alpha}$ and $\tilde{Y}$ equal α and Y, respectively, with the j_0th component removed.

III.1.2 Approximations by Means of Local Scaled Short-Range Interactions

The operator $-\Delta_{\alpha,Y}$ of Sect 1.1 represents an idealization in the sense that the interaction at each center has zero-range. It is therefore natural to ask in what sense this idealization represents the asymptotic behavior when the range of the interaction diminishes.

We will prove in Theorem 1.2.1 that $-\Delta_{\alpha,Y}$ is approximated in norm resolvent sense by operators with short-range interactions. Since our ultimate goal in this chapter is to model regular structures, e.g., crystals, we shall assume that the approximating operator has only a finite number of different potentials, viz.

$$H_{\varepsilon,Y} = -\Delta \dotplus \varepsilon^{-2} \sum_{j=1}^{\infty} \lambda_j(\varepsilon) V_j((\cdot - y_j)/\varepsilon), \qquad \varepsilon > 0, \tag{1.2.1}$$

where

$$V_j \in \{W_1, \ldots, W_N\}, \qquad \lambda_j(\varepsilon) \in \{\mu_1(\varepsilon), \ldots, \mu_N(\varepsilon)\}, \qquad j \in \mathbb{N}. \tag{1.2.2}$$

First, we derive an explicit expression for the resolvent of $H_{\varepsilon,Y}$. To this end, we need some definitions. Let

$$\mathscr{H} = \bigoplus_{j=1}^{\infty} L^2(\mathbb{R}^3) \tag{1.2.3}$$

and

$$\begin{aligned} &A_\varepsilon(k): \mathscr{H} \to L^2(\mathbb{R}^3), \\ &B_\varepsilon(k): \mathscr{H} \to \mathscr{H}, \\ &C_\varepsilon(k): L^2(\mathbb{R}^3) \to \mathscr{H}, \end{aligned} \tag{1.2.4}$$

be bounded operators with integral kernels

$$\begin{aligned} &A_{\varepsilon,j}(k, x, x') = G_k(x - \varepsilon x' - y_j)v_j(x'), \\ &B_{\varepsilon,jj'}(k, x, x') = \begin{cases} \varepsilon\lambda_j(\varepsilon)u_j(x)G_k(\varepsilon(x - x') + y_j - y_{j'})v_{j'}(x'), & j \neq j', \\ \lambda_j(\varepsilon)u_j(x)G_{\varepsilon k}(x - x')v_j(x'), & j = j', \end{cases} \\ &C_{\varepsilon,j}(k, x, x') = \lambda_j(\varepsilon)u_j(x)G_k(\varepsilon x + y_j - x'); \qquad \operatorname{Im} k > 0, \quad \varepsilon \geq 0, \quad j, j' \in \mathbb{N}. \end{aligned} \tag{1.2.5}$$

Theorem 1.2.1. *Let $W_j \in R$, supp W_j compact, be real-valued and let $\mu_j(\varepsilon) = 1 + \varepsilon\mu_j'(0) + o(\varepsilon)$ as $\varepsilon \downarrow 0$, $j = 1, \ldots, N$. Assume, furthermore, that $Y = \{y_j \in \mathbb{R}^3 \mid j \in \mathbb{N}\}$ satisfies $|y_j - y_{j'}| \geq d > 0$, $j \neq j'$, $j, j' \in \mathbb{N}$. Then the self-adjoint operator in $L^2(\mathbb{R}^3)$*

$$H_{\varepsilon,Y} = -\Delta \dotplus \varepsilon^{-2} \sum_{j=1}^{\infty} \lambda_j(\varepsilon) V_j((\cdot - y_j)/\varepsilon), \tag{1.2.6}$$

where

$$\lambda_j \in \{\mu_1, \ldots, \mu_N\}, \qquad V_j \in \{W_1, \ldots, W_N\}, \qquad j \in \mathbb{N}, \tag{1.2.7}$$

has the resolvent

$$(H_{\varepsilon,Y} - k^2)^{-1} = G_k - \varepsilon A_\varepsilon(k)[1 + B_\varepsilon(k)]^{-1}C_\varepsilon(k),$$
$$k^2 \in \rho(H_{\varepsilon,Y}), \quad \operatorname{Im} k > 0. \tag{1.2.8}$$

Assume that $\lambda_j'(0) \neq 0$ if $H_j = -\Delta \dotplus V_j$ is in case III *or* IV. *Then $H_{\varepsilon,Y}$ converges in norm resolvent sense to the operator $-\Delta_{\alpha,Y}$ defined by* (1.1.6), *i.e.,*

$$\underset{\varepsilon\downarrow 0}{\text{n-lim}}\, (H_{\varepsilon,Y} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \tag{1.2.9}$$

where $\alpha = \{\alpha_j\}_{j\in\mathbb{N}}$ and α_j equals

$$\alpha_j = \begin{cases} \infty & \text{in case I}, \\ -\lambda_j'(0)\,|(v_j, \phi_j)|^{-2} & \text{in case II}, \\ \infty & \text{in case III}, \\ -\lambda_j'(0)\left\{\sum_{l=1}^{N_j} |(v_j, \phi_{jl})|^2\right\}^{-1} & \text{in case IV}; \qquad j \in \mathbb{N}. \end{cases} \tag{1.2.10}$$

PROOF. Using Theorem C.4 we know that the self-adjoint operator

$$H_Y(\varepsilon) = -\Delta \dotplus \sum_{j=1}^{\infty} \lambda_j(\varepsilon) V_j(\cdot - \varepsilon^{-1}y_j) \tag{1.2.11}$$

has the resolvent

$$(H_Y(\varepsilon) - k^2)^{-1} = G_k - \tilde{A}_\varepsilon(k)[1 + \tilde{B}_\varepsilon(k)]^{-1}\tilde{C}_\varepsilon(k), \qquad k^2 \in \rho(H_y(\varepsilon)), \quad \operatorname{Im} k > 0, \tag{1.2.12}$$

where

$$\begin{aligned} &\tilde{A}_\varepsilon(k)\colon \mathscr{H} \to L^2(\mathbb{R}^3), && \tilde{A}_\varepsilon(k) = [G_k \tilde{v}_j]_{j \in \mathbb{N}}, \\ &\tilde{B}_\varepsilon(k)\colon \mathscr{H} \to \mathscr{H}, && \tilde{B}_\varepsilon(k) = [\lambda_j(\varepsilon)\tilde{u}_j G_k \tilde{v}_{j'}]_{j,j' \in \mathbb{N}}, \\ &\tilde{C}_\varepsilon(k)\colon L^2(\mathbb{R}^3) \to \mathscr{H}, && \tilde{C}_\varepsilon(k) = [\lambda_j(\varepsilon)\tilde{u}_j G_k]_{j \in \mathbb{N}}; \qquad \varepsilon > 0, \quad \operatorname{Im} k > 0, \end{aligned} \tag{1.2.13}$$

are bounded operators with $\tilde{u}_j$, $\tilde{v}_j$ defined by (II.1.2.11). Introducing the scaling operator U_ε (cf. (II.1.2.3)) and the translation operator T_y (cf. (II.1.2.13)) as in the proof of Lemma II.1.2.2 we obtain (1.2.8). Next we need the limits of the operators $A_\varepsilon(k)$, $C_\varepsilon(k)$, and $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ as $\varepsilon \downarrow 0$. As in Theorem II.1.2.1, $A_\varepsilon(k)$ and $C_\varepsilon(k)$ have natural candidates for their limits, while the limit of $\varepsilon[1 + B_\varepsilon(k)]^{-1}$ is more involved. Starting with the operator $C_\varepsilon(k)$ (taking $\lambda_j(\varepsilon) \equiv 1$ for simplicity) we have that

$$\begin{aligned} &\sum_{j=1}^{\infty} \|[C_{\varepsilon,j}(k) - C_{0,j}(k)]f\|^2 \\ &\quad = \sum_{j=1}^{\infty} \int_{\mathbb{R}^3} d^3x\, |V_j(x)| \left| \int_{\mathbb{R}^3} d^3x' \left[\frac{e^{ik|\varepsilon x + y_j - x'|}}{4\pi|\varepsilon x + y_j - x'|} - \frac{e^{ik|y_j - x'|}}{4\pi|y_j - x'|} \right] f(x') \right|^2 \\ &\quad \le \int_{\mathbb{R}^3} d^3x\, W(x) \sum_{j=1}^{\infty} \left[\int_{\mathbb{R}^3} d^3x' \left| \frac{e^{ik|\varepsilon x + y_j - x'|}}{4\pi|\varepsilon x + y_j - x'|} - \frac{e^{ik|y_j - x'|}}{4\pi|y_j - x'|} \right|^2 e^{\operatorname{Im} k|y_j - x'|}\,. \right. \\ &\qquad \left. \cdot \int_{\mathbb{R}^3} d^3x''\, e^{-\operatorname{Im} k|y_j - x''|} |f(x'')|^2 \right. \\ &\quad \le c \left[\int_{\mathbb{R}^3} d^3x\, W(x) \int_{\mathbb{R}^3} d^3x' \left| \frac{e^{ik|\varepsilon x - x'|}}{4\pi|\varepsilon x - x'|} - \frac{e^{ik|x'|}}{4\pi|x'|} \right|^2 e^{\operatorname{Im} k|x'|} \right] \|f\|^2, \\ &\hspace{22em} f \in L^2(\mathbb{R}^3), \end{aligned} \tag{1.2.14}$$

where

$$c = \sup_{x \in \mathbb{R}^3} \sum_{j=1}^{\infty} e^{-\operatorname{Im} k|y_j - x|} \quad \text{and} \quad W(x) = \sum_{j=1}^{N} |W_j(x)|.$$

Using the dominated convergence theorem we see that the right-hand side is bounded by $c(\varepsilon)\|f\|^2$ where $c(\varepsilon) \to 0$ as $\varepsilon \downarrow 0$, proving the assertion for $C_\varepsilon(k)$. Similarly, one shows that $A_\varepsilon(k)^* \to A_0(k)^*$ in norm as $\varepsilon \downarrow 0$. Writing

$$1 + B_\varepsilon(k) = 1 + D_\varepsilon(k) + \varepsilon E_\varepsilon(k), \tag{1.2.15}$$

where

$$\begin{aligned} D_\varepsilon(k) &= [\delta_{jj'}\lambda_j(\varepsilon) u_j G_k v_j]_{j,j' \in \mathbb{N}}, \\ E_\varepsilon(k) &= [(1 - \delta_{jj'})\varepsilon^{-1} B_{\varepsilon,jj'}(k)]_{j,j' \in \mathbb{N}}, \end{aligned} \tag{1.2.16}$$

we infer from

$$\varepsilon[1 + B_\varepsilon(k)]^{-1} = \{1 + \varepsilon[1 + D_\varepsilon(k)]^{-1} E_\varepsilon(k)\}^{-1} \varepsilon[1 + D_\varepsilon(k)]^{-1} \tag{1.2.17}$$

that it suffices to determine the limits of $\varepsilon[1 + D_\varepsilon(k)]^{-1}$ and $E_\varepsilon(k)$ as $\varepsilon \downarrow 0$. Estimating

$\|E_\varepsilon(k) - E_0(k)\|$ using Lemma C.3 we only need to prove that

$$\sup_{j\in\mathbb{N}} \sum_{\substack{j'=1\\ j'\neq j}}^{\infty} \int_{\mathbb{R}^6} d^3x\, d^3x'\, W(x)W(x')\left|\frac{e^{ik|\varepsilon(x-x')+y_j-y_{j'}|}}{|\varepsilon(x-x')+y_j-y_{j'}|} - \frac{e^{ik|y_j-y_{j'}|}}{|y_j-y_{j'}|}\right|^2 \xrightarrow[\varepsilon\downarrow 0]{} 0. \tag{1.2.18}$$

This, however, follows using the dominated convergence theorem. The matrix $\varepsilon[1 + D_\varepsilon(k)]^{-1}$ is diagonal, and for each entry on the diagonal we know the limit from the one-center case, Lemma I.1.2.4. Since we only have a finite number of different potentials, the limit is uniform on the diagonal and hence also exists in $\mathscr{H}$. Thus

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} \varepsilon[1 + D_\varepsilon(k)]^{-1} = [\delta_{jj'}\tilde{D}(k)_j]_{j,j'\in\mathbb{N}}, \tag{1.2.19}$$

where

$$\tilde{D}(k)_j = \begin{cases} 0 & \text{in case I,} \\ [(4\pi)^{-1}ik|(v_j, \phi_j)|^2 + \lambda_j'(0)]^{-1}(\tilde{\phi}_j, \cdot)\phi_j & \text{in case II,} \\ [\lambda_j'(0)]^{-1} \sum_{l=1}^{N_j} (\tilde{\phi}_{jl'}, \cdot)\phi_{jl} & \text{in case III,} \\ \sum_{l,l'=1}^{N_j} (\tilde{\phi}_j, B_{j1}(k)\phi_j)^{-1}_{ll'}(\tilde{\phi}_{jl'}, \cdot)\phi_{jl} & \text{in case IV,} \end{cases} \tag{1.2.20}$$

with $(\tilde{\phi}_j, B_{j1}(k)\phi_j)^{-1}_{ll'}$ defined as in Lemma I.1.2.4 with V replaced by V_j and with α_j defined according to (1.2.10). Having found all the necessary limits, a similar computation as in the proof of Theorem II.1.2.1 yields the assertions claimed. ■

III.1.3 Periodic Point Interactions

One of the most interesting special cases of the model constructed in Sect. 1.1 occurs when Y and α are periodic. We then obtain the so-called *one-electron model of a solid* which is based on the following assumptions (A)–(E):

(A) The solid is supposed to consist of a fixed number of heavy nuclei arranged in a regular lattice surrounded by core electrons. Each nucleus has the same number of core electrons such that the whole system is neutral.

Although it is not proved from first principles that a neutral system consisting of heavy nuclei and electrons, interacting via the Coulomb interaction, forms a regular or approximately regular lattice as the ground state, it is nevertheless an observed fact in nature that solids consist of nuclei arranged in regular structures. This makes assumption (A) a reasonable starting point to investigate properties of solids. Hence the solid is assumed to consist of an electron gas immersed in a background of positive ions arranged in a regular lattice.

(B) The electron–electron interactions are neglected, only interactions between the electrons and the heavy nuclei are taken into account.

From an ideal point of view one would, of course, like to solve the many-body problem using only assumption (A). However, many-body problems of the above type are presently beyond the scope of an analytical treatment. The validity of assumption (B) can be further enhanced by replacing the atomic potential by an averaged potential, and the electron mass by an effective mass. In addition, it is experimentally verified that the electrons move nearly free in a metal thus making assumption (B) a reasonable one.

(C) The solid is assumed to be infinitely extended, and each nucleus gives rise to the same potential.

Assumption (C) is a mathematical device to obtain a strictly periodic, not only approximately periodic, interaction, and it is reasonable because the solid consists of the order of 10^{23} nuclei. Clearly, this assumption disregards surface effects. Furthermore, the complete periodicity does not allow one to study various defects, dislocations, and impurities. Nevertheless, by perturbing the periodic Hamiltonian we will be able to study various kinds of impurities, see Sects. 1.9 and 2.6 and Ch. 5.

(D) All "higher-order" effects are neglected, e.g., relativistic effects, lattice vibrations, spin–orbit coupling, electron–phonon interactions ([332]).

Clearly, all these effects play a role in realistic systems. Hypothesis (D) is the price one pays for a rigorous analytical treatment.

From assumptions (A)–(D) it follows that we have to study the "usual" Schrödinger operator which reads, in appropriate units,

$$H = -\Delta + V, \tag{1.3.1}$$

where the potential V is periodic, viz.

$$V(x + \lambda) = V(x), \qquad x \in \mathbb{R}^3, \quad \lambda \in \Lambda, \tag{1.3.2}$$

Λ being the underlying lattice. By definition (1.3.1) and (1.3.2) constitute the one-electron model of an infinite, perfect solid.

To obtain a solvable model we will introduce our last assumption, namely:

(E) Assume that formally

$$V(x) = -\sum_{\lambda \in \Lambda} \mu\delta(x - \lambda). \tag{1.3.3}$$

The atomic potential is of Coulomb type and thus has a singularity at each point of the lattice and in particular is of long range. However, as we mentioned in the comments to assumption (B), the actual potential has to be replaced by an averaged potential which qualitatively looks like the one in Figure 4 in one dimension. Thus it has a singularity at each lattice point and is approximately constant in between. By replacing the singularity with a δ-function and the constant value by zero we obtain (1.3.3) which is a particular example of a so-called muffin-tin potential.

We will also be able to solve the problem where we allow a finite number of different nuclei in each primitive cell $\hat{\Gamma}$ (for the definition of $\hat{\Gamma}$, see the next section), i.e.,

$$V(x) = -\sum_{j=1}^{N} \sum_{\lambda \in \Lambda} \mu_j \delta(x - \lambda - y_j), \tag{1.3.4}$$

where $\{y_1, \ldots, y_N\} \subset \hat{\Gamma}$. This provides a model of a multiatomic crystal or an ordered alloy.

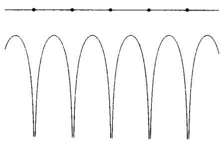


Figure 4

Finally, by allowing Λ to be one- or two-dimensional lattices embedded in $\mathbb{R}^3$ we obtain the one-electron models of an infinite straight polymer and an infinite monomolecular layer, respectively.

III.1.4 Crystals

The first regular structure to be considered is the full infinite crystal in three dimensions. Before we start with explicit computations for the point interaction Hamiltonian, it will be instructive to study on a formal level what sort of properties one should expect in general with a Schrödinger operator

$$H = -\Delta + V \tag{1.4.1}$$

in $L^2(\mathbb{R}^3)$ where the real-valued potential V is a smooth periodic function, i.e.,

$$V(x + \lambda) = V(x), \qquad x \in \mathbb{R}^3, \quad \lambda \in \Lambda, \tag{1.4.2}$$

and where Λ is a *Bravais lattice*,

$$\Lambda = \{n_1 a_1 + n_2 a_2 + n_3 a_3 \in \mathbb{R}^3 | (n_1, n_2, n_3) \in \mathbb{Z}^3\} \tag{1.4.3}$$

and a_1, a_2, a_3 is a basis in $\mathbb{R}^3$. This will also allow us to introduce the basic nomenclature. The *basic periodic cell* or *primitive cell* $\hat{\Gamma}$ is mathematically

$$\hat{\Gamma} = \mathbb{R}^3/\Lambda \tag{1.4.4}$$

and can be identified with the *Wigner–Seitz cell*

$$\hat{\Gamma} = \{s_1 a_1 + s_2 a_2 + s_3 a_3 \in \mathbb{R}^3 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2, 3\}. \tag{1.4.5}$$

Since V is periodic, it can be expanded in a Fourier series, i.e.,

$$V(x) = \sum_{\gamma \in \Gamma} V_\gamma e^{i\gamma x}, \tag{1.4.6}$$

where

$$V_\gamma = |\hat{\Gamma}|^{-1} \int_{\hat{\Gamma}} d^3 v \; V(v) e^{-i\gamma v} \tag{1.4.7}$$

and Γ equals the *dual lattice* (or *orthogonal lattice* or *reciprocal lattice*),

$$\Gamma = \{n_1 b_1 + n_2 b_2 + n_3 b_3 \in \mathbb{R}^3 | (n_1, n_2, n_3) \in \mathbb{Z}^3\}, \tag{1.4.8}$$

where the *dual basis* b_1, b_2, b_3 satisfies

$$a_j b_{j'} = 2\pi \delta_{jj'}, \qquad j, j' = 1, 2, 3. \tag{1.4.9}$$

It will be useful to consider H in p-space, thus we make a Fourier transform of H. We then obtain

$$\hat{H} = \mathscr{F} H \mathscr{F}^{-1} = p^2 + (2\pi)^{-3/2} \overline{(\hat{V}(p - \cdot), \cdot)} \tag{1.4.10}$$

which is a formal way of writing the operator

$$(\hat{H}\hat{f})(p) = p^2 \hat{f}(p) + (2\pi)^{-3/2} \int_{\mathbb{R}^3} d^3 q \, \hat{V}(p - q) \hat{f}(q). \tag{1.4.11}$$

Using the Fourier inversion formula

$$V(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} d^3 p \, \hat{V}(p) e^{ipx} \tag{1.4.12}$$

one formally would expect

$$\hat{V}(p) = (2\pi)^{3/2} \sum_{\gamma \in \Gamma} V_\gamma \delta(p - \gamma), \tag{1.4.13}$$

since then

$$\begin{aligned} (2\pi)^{-3/2} \int_{\mathbb{R}^3} d^3 p \, \hat{V}(p) e^{ipx} &= \sum_{\gamma \in \Gamma} V_\gamma \int_{\mathbb{R}^3} d^3 p \, \delta(p - \gamma) e^{ipx} \\ &= \sum_{\gamma \in \Gamma} V_\gamma e^{i\gamma x} = V(x) \end{aligned} \tag{1.4.14}$$

which is (1.4.6).

Inserting (1.4.13) into (1.4.10) we see that $\hat{H}$ formally can be written

$$\hat{H} = p^2 + \sum_{\gamma \in \Gamma} V_\gamma (\delta(p - \gamma - \cdot), \cdot). \tag{1.4.15}$$

This makes it natural to decompose the Hilbert space $L^2(\mathbb{R}^3)$ according to

$$\begin{aligned} &\mathscr{U}: L^2(\mathbb{R}^3) \to L^2(\hat{\Lambda}, l^2(\Gamma)) \equiv \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, l^2(\Gamma), \\ &(\mathscr{U}\hat{f})(\theta, \gamma) = \hat{f}(\gamma + \theta), \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad \hat{f} \in L^2(\mathbb{R}^3), \end{aligned} \tag{1.4.16}$$

where $\hat{\Lambda}$ is the *dual group of* Λ (or *basic periodic cell* or *primitive cell of the dual lattice* Γ), i.e.,

$$\hat{\Lambda} = \mathbb{R}^3/\Gamma. \tag{1.4.17}$$

By identifying $\hat{\Lambda}$ with the Wigner–Seitz cell of the dual lattice Γ (defined correspondingly to (1.4.5)) we obtain the important concept of the *Brillouin zone*, namely

$$\hat{\Lambda} = \{s_1 b_1 + s_2 b_2 + s_3 b_3 \in \mathbb{R}^3 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2, 3\}. \tag{1.4.18}$$

Thus the decomposition simply corresponds to writing a vector $p \in \mathbb{R}^3$ uniquely in the form

$$p = \theta + \gamma, \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma. \tag{1.4.19}$$

This decomposition of $L^2(\mathbb{R}^3)$ will, of course, also decompose the Schrödinger operator $\hat{H}$ which we now write as

$$\mathscr{U}\hat{H}\mathscr{U}^{-1} = \int_{\hat{\Lambda}}^{\oplus} d^3\theta\, \hat{H}(\theta), \tag{1.4.20}$$

where $\hat{H}(\theta)$ acts on $l^2(\Gamma)$ according to

$$(\hat{H}(\theta)g)(\gamma) = |\gamma + \theta|^2 g(\gamma) + \sum_{\gamma' \in \Gamma} V_{\gamma'} g(\gamma - \gamma'), \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l^2(\Gamma). \tag{1.4.21}$$

Thus (1.4.20) simply means

$$(\mathscr{U}\hat{H}\mathscr{U}^{-1}\hat{f})(\theta, \gamma) = (\hat{H}(\theta)\hat{f}(\theta, \cdot))(\gamma), \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad \hat{f} \in L^2(\hat{\Lambda}, l^2(\Gamma)). \tag{1.4.22}$$

In order to study the spectrum of $\hat{H}$, and hence of H, we have to study the spectrum of $\hat{H}(\theta)$. Since the free decomposed Hamiltonian $-\hat{\Delta}(\theta)$ (i.e., $V_\gamma = 0$ for all $\gamma \in \Gamma$) has a purely discrete spectrum, namely

$$\sigma(-\hat{\Delta}(\theta)) = \sigma_{\mathrm{d}}(-\hat{\Delta}(\theta)) = |\Gamma + \theta|^2, \tag{1.4.23}$$

where

$$|\Gamma + \theta|^2 = \{|\gamma + \theta|^2 \in \mathbb{R} \,|\, \gamma \in \Gamma\}, \qquad \theta \in \hat{\Lambda}; \tag{1.4.24}$$

$\hat{H}(\theta)$ will also have a purely discrete spectrum consisting of isolated eigenvalues of finite multiplicity. As θ varies in $\hat{\Lambda}$, the Brillouin zone, the eigenvalues will broaden to form bands if the dependence in θ is smooth. Hence

$$\sigma(H) = \sigma(\hat{H}) = \bigcup_{\theta \in \hat{\Lambda}} \sigma(\hat{H}(\theta)) \tag{1.4.25}$$

which means that the spectrum of Schrödinger operators with periodic potentials consists of bands, which may or may not be separated by gaps.

We will now implement the point interaction Hamiltonian into this framework. There are essentially two ways of doing this. First, we could take the operator $-\hat{\Delta}_{\alpha, Y}$ from Sect. 1.1, make α and Y periodic and perform the direct integral decomposition (1.4.20). Second, we could start with the unperturbed decomposed Hamiltonian $-\hat{\Delta}(\theta)$ given by (1.4.21) with $V_\gamma = 0$ for all $\gamma \in \Gamma$ and then perturb it with point interactions in the spirit of Theorem II.1.1.1. This makes the approach independent of the technical Theorem 1.1.1, but raises the consistency problem (since we have to make a renormalization to pass from μ's to α's): Do the two approaches yield the same operator? We will follow the latter approach as this makes the presentation independent of Part II, but for completeness we will also prove that the two approaches lead to the same operator.

Our potential will then be, formally

$$V(x) = -\sum_{j=1}^{N} \sum_{\lambda \in \Lambda} \mu_j \delta(x - y_j - \lambda), \qquad \mu_j \in \mathbb{R}, \quad j = 1, \dots, N, \quad (1.4.26)$$

when we allow interactions at a finite number of points $y_1, \dots, y_N$ in the basic periodic cell $\hat{\Gamma}$,

$$Y = \{y_1, \dots, y_N\} \subset \hat{\Gamma}. \qquad (1.4.27)$$

Then

$$V_\gamma = |\hat{\Gamma}|^{-1} \int_{\hat{\Lambda}} d^3v\, V(v) e^{-i\gamma v} = -|\hat{\Gamma}|^{-1} \sum_{j=1}^{N} \mu_j e^{-i\gamma y_j}, \qquad \gamma \in \Gamma. \quad (1.4.28)$$

Inserting this into (1.4.21) we formally obtain

$$\begin{aligned}(\hat{H}(\theta)g)(\gamma) &= |\gamma + \theta|^2 g(\gamma) - |\hat{\Gamma}|^{-1} \sum_{\gamma' \in \Gamma} \sum_{j=1}^{N} \mu_j e^{-i\gamma' y_j} g(\gamma - \gamma') \\ &= |\gamma + \theta|^2 g(\gamma) - |\hat{\Gamma}|^{-1} \sum_{j=1}^{N} \left[\mu_j e^{-i\gamma y_j} \sum_{\gamma' \in \Gamma} e^{i\gamma' y_j} g(\gamma') \right], \\ &\qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l_0(\Gamma). \quad (1.4.29)\end{aligned}$$

As this of course does not define a self-adjoint operator in $l^2(\Gamma)$ we introduce the operators

$$(\hat{H}^\omega(\theta)g)(\gamma) = |\gamma + \theta|^2 g(\gamma) - |\hat{\Gamma}|^{-1} \sum_{j=1}^{N} \mu_j(\omega)(\phi_{y_j}^\omega(\theta), g)\phi_{y_j}^\omega(\theta),$$
$$\theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l_0(\Gamma), \quad \omega > 0, \quad (1.4.30)$$

where $(\cdot, \cdot)$ is the inner-product in $l^2(\Gamma)$ and $\phi_{y_j}^\omega(\theta)$ equals the function

$$\phi_{y_j}^\omega(\theta, \gamma) = \chi_\omega(\gamma + \theta) e^{-i(\gamma + \theta)y_j}, \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad j = 1, \dots, N, \quad (1.4.31)$$

and χ_ω, as usual, denotes the characteristic function of the closed ball in $\mathbb{R}^3$ with radius $\omega > 0$ and center at the origin.

With this operator we can state the following

Theorem 1.4.1. *Let $\hat{H}^\omega(\theta)$ be the self-adjoint operator in $l^2(\Gamma)$ given by* (1.4.30) *with domain*

$$\mathcal{D}(\hat{H}^\omega(\theta)) = \mathcal{D}(-\hat{\Delta}(\theta)) = \left\{ g \in l^2(\Gamma) \,\middle|\, \sum_{\gamma \in \Gamma} |\gamma + \theta|^4 |g(\gamma)|^2 < \infty \right\}, \qquad \theta \in \hat{\Lambda}. \quad (1.4.32)$$

If

$$\mu_j(\omega) = \left(\alpha_j + \frac{\omega}{2\pi^2} \right)^{-1}, \qquad \alpha_j \in \mathbb{R}, \quad j = 1, \dots, N, \quad \omega > 0, \quad (1.4.33)$$

then $\hat{H}^\omega(\theta)$ converges for all $\theta \in \hat{\Lambda}$ in norm resolvent sense as $\omega \to \infty$ to a self-adjoint operator which we denote by $-\hat{\Delta}_{\alpha, \Lambda, Y}(\theta)$. The resolvent of $-\hat{\Delta}_{\alpha, \Lambda, Y}(\theta)$

reads

$$(-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}$$
$$= G_k(\theta) + |\hat{\Gamma}|^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]_{jj'}^{-1} (F_{-\bar{k},y_{j'}}(\theta), \cdot) F_{k,y_j}(\theta),$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \det[\Gamma_{\alpha,\Lambda,Y}(k,\theta)] \neq 0,$$
$$\theta \in \hat{\Lambda}, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j = 1, \ldots, N, \qquad (1.4.34)$$

where

$$\alpha = (\alpha_1, \ldots, \alpha_N), \qquad Y = (y_1, \ldots, y_N) \subseteq \hat{\Gamma} \qquad (1.4.35)$$

and

$$\Gamma_{\alpha,\Lambda,Y}(k,\theta) = [\alpha_j \delta_{jj'} - g_k(y_j - y_{j'}, \theta)]_{j,j'=1}^{N},$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \qquad (1.4.36)$$

and

$$g_k(x,\theta)$$
$$= \begin{cases} |\hat{\Gamma}|^{-1} \lim\limits_{\omega\to\infty} \sum\limits_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\leq\omega}} \dfrac{e^{i(\gamma+\theta)x}}{|\gamma+\theta|^2 - k^2}, & x \in \mathbb{R}^3 - \Lambda, \\ (2\pi)^{-3} e^{-i\theta x} \lim\limits_{\omega\to\infty} \left[\sum\limits_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\leq\omega}} \dfrac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - 4\pi\omega \right], & x \in \Lambda, \end{cases}$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}. \qquad (1.4.37)$$

If $\operatorname{Im} k > 0$, *then* $g_k(x,\theta)$ *also equals*

$$g_k(x,\theta) = \begin{cases} \sum\limits_{\lambda\in\Lambda} G_k(x+\lambda) e^{-i\theta\lambda}, & x \in \mathbb{R}^3 - \Lambda, \\ \sum\limits_{\lambda\in\Lambda} \tilde{G}_k(x+\lambda) e^{-i\theta\lambda} + \dfrac{ik}{4\pi}, & x \in \Lambda, \quad \theta \in \hat{\Lambda}, \end{cases} \qquad (1.4.38)$$

(*cf.* (II.1.1.26)). *Furthermore,*

$$F_{k,y_j}(\theta,\gamma) = \frac{e^{-i(\gamma+\theta)y_j}}{|\gamma+\theta|^2 - k^2},$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \quad j = 1, \ldots, N, \qquad (1.4.39)$$

and $G_k(\theta)$ *is the multiplication operator in* $l^2(\Gamma)$ *with the function* $(|\gamma + \theta|^2 - k^2)^{-1}$, *i.e.*,

$$G_k(\theta): l^2(\Gamma) \to l^2(\Gamma),$$
$$G_k(\theta)g)(\gamma) = (|\gamma+\theta|^2 - k^2)^{-1} g(\gamma), \qquad (1.4.40)$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l^2(\Gamma).$$

Proof. From Lemma B.5 we know that

$$(\hat{H}^\omega(\theta) - k^2)^{-1} = G_k(\theta) + \sum_{j,j'=1}^{N} [\Gamma^\omega_{\Lambda,Y}(k,\theta)]^{-1}_{jj'}(G_{-\bar{k}}(\theta)\phi^\omega_{y_{j'}}(\theta), \cdot)G_k(\theta)\phi^\omega_{y_j},$$
$$\det[\Gamma^\omega_{\Lambda,Y}(k,\theta)] \neq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k > 0, \quad \theta \in \hat{\Lambda},$$
$$\Gamma^\omega_{\Lambda,Y}(k,\theta) = [|\hat{\Gamma}|\mu_j(\omega)^{-1}\delta_{jj'} - (\phi^\omega_{y_j}(\theta), G_k(\theta)\phi^\omega_{y_{j'}}(\theta))]^N_{j,j'=1}. \quad (1.4.41)$$

The jth diagonal entry of the matrix $\Gamma^\omega_{\Lambda,Y}(k,\theta)$ equals

$$|\hat{\Gamma}|\mu_j(\omega)^{-1} - (\phi^\omega_{y_j}(\theta), G_k(\theta)\phi^\omega_{y_j}(\theta)) = |\hat{\Gamma}|\mu_j(\omega)^{-1} - \sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\leq\omega}} \frac{1}{|\gamma+\theta|^2 - k^2},$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0. \quad (1.4.42)$$

To estimate the divergence of this series as $\omega \to \infty$ is more difficult than to isolate the corresponding divergence in the finite center case, Theorem II.1.1.1, since we are not able to obtain the partial sum of this series in a closed form. However, by applying the Poisson summation formula this sum can be controlled. Using Lemma 1.4.2, proved after this theorem, we infer that

$$|\hat{\Gamma}|\mu_j(\omega)^{-1} - \sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\leq\omega}} \frac{1}{|\gamma+\theta|^2 - k^2}$$
$$= |\hat{\Gamma}|\left[\alpha_j - (2\pi)^{-3}\left(\sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\leq\omega}} \frac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - 4\pi\omega\right)\right],$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad (1.4.43)$$

converges as $\omega \to \infty$ to $|\hat{\Gamma}|[\alpha_j - g_k(0,\theta)]$ where $g_k(0,\theta)$ is given by (1.4.37). The off-diagonal elements of the matrix converge, viz.

$$(\phi^\omega_{y_j}(\theta), G_k(\theta)\phi^\omega_{y_{j'}}(\theta)) = \sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\leq\omega}} \frac{e^{i(\gamma+\theta)(y_j - y_{j'})}}{|\gamma+\theta|^2 - k^2} \xrightarrow[\omega\to\infty]{} |\hat{\Gamma}|g_k(y_j - y_{j'}, \theta),$$
$$j \neq j', \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad (1.4.44)$$

using Lemma 1.4.2 again. A straightforward computation shows that

$$\|(G_{-\bar{k}}(\theta)\phi^\omega_{y_{j'}}(\theta), \cdot)G_k(\theta)\phi^\omega_{y_j}(\omega) - (F_{-\bar{k},y_{j'}}(\theta), \cdot)F_{k,y_j}(\theta)\|_2 \xrightarrow[\omega\to\infty]{} 0. \quad (1.4.45)$$

Hence we conclude

$$\operatorname*{n-lim}_{\omega\to\infty} (\hat{H}^\omega(\theta) - k^2)^{-1} = G_k(\theta) + |\hat{\Gamma}|^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]^{-1}_{jj'}(F_{-\bar{k},y_{j'}}(\theta), \cdot)F_{k,y_j}(\theta) \quad (1.4.46)$$

for k^2 sufficiently negative. To conclude that the right-hand side of (1.4.46) is the resolvent of a self-adjoint operator $-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)$ is similar to that of Theorem II.1.1.1 and hence will be omitted. The equivalence of (1.4.37) and (1.4.38) when $\operatorname{Im} k > 0$ is precisely the content of Lemma 1.4.2. ∎

We did not use the full content of Lemma 1.4.2, but only the fact that (1.4.44) converges conditionally and that

$$\sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\le\omega}}\frac{|\hat{\Lambda}|}{|\gamma+\theta|^2-k^2}=4\pi\omega+O(1)\quad\text{as }\omega\to\infty,$$

which also can be proved directly. However, for the consistency result in Theorem 1.4.3, we also need the alternative expressions for the sums which are contained in Lemma 1.4.2.

Lemma 1.4.2 (Poisson Summation Formula). *Let $k^2\in\mathbb{C}$, $\operatorname{Im} k>0$, $a\in\mathbb{R}^3$, and $\theta\in\hat{\Lambda}$. Then*

$$\sum_{\substack{\lambda\in\Lambda\\\lambda\ne-a}}\frac{e^{ik|\lambda+a|}}{4\pi|\lambda+a|}e^{-i\theta\lambda}$$

$$=\begin{cases}|\hat{\Gamma}|^{-1}\lim\limits_{\omega\to\infty}\sum\limits_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\le\omega}}\dfrac{e^{i(\gamma+\theta)a}}{|\gamma+\theta|^2-k^2}, & a\in\mathbb{R}^3-\Lambda,\\[2ex](2\pi)^{-3}e^{i\theta a}\lim\limits_{\omega\to\infty}\left[\sum\limits_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\le\omega}}\dfrac{|\hat{\Lambda}|}{|\gamma+\theta|^2-k^2}-4\pi\omega\right]-\dfrac{ik}{4\pi}, & a\in\Lambda.\end{cases}\tag{1.4.47}$$

PROOF. Formally eq. (1.4.47) is essentially the Poisson summation formula for the function $G_k(x)$. However, due to the poor convergence (or actually divergence without renormalization when $a\in\Lambda$), special care is needed. First, we treat the most singular case, i.e., when $a\in\Lambda$. Due to the invariance modulo Λ it suffices to consider $a=0$. Let

$$f(\omega)=\sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\le\omega}}\frac{1}{|\gamma+\theta|^2-k^2},\qquad\omega\ge0,\tag{1.4.48}$$

($k^2\in\mathbb{C}$, $\operatorname{Im} k>0$, and $\theta\in\hat{\Lambda}$ will be fixed during the calculations and are therefore omitted in the notation). Then f is a step function, $f(\omega)\to\infty$ as $\omega\to\infty$, $f(0)=0$. Define

$$F(\eta)=\int_0^\infty e^{-\eta\omega}\,df(\omega)=\sum_{\gamma\in\Gamma}\frac{e^{-\eta|\gamma+\theta|}}{|\gamma+\theta|^2-k^2},\qquad\eta>0.\tag{1.4.49}$$

Applying now the Poisson summation formula ([94], Theorem 67 and eq. (19), p. 260) we obtain

$$\begin{aligned}F(\eta)&=|\hat{\Lambda}|^{-1}\left[\int_{\mathbb{R}^3}d^3x\,G_k(x)\frac{8\pi\eta}{(x^2+\eta^2)^2}+\sum_{\substack{\lambda\in\Lambda\\\lambda\ne0}}e^{-i\theta\lambda}\int_{\mathbb{R}^3}d^3x\,G_k(\lambda-x)\frac{8\pi\eta}{(x^2+\eta^2)^2}\right]\\&=|\hat{\Lambda}|^{-1}\left[\int_{\mathbb{R}^3}d^3p\frac{e^{-\eta|p|}}{p^2-k^2}+(2\pi)^3\sum_{\substack{\lambda\in\Lambda\\\lambda\ne0}}e^{-i\theta\lambda}\int_{\mathbb{R}^3}d^3x\frac{G_k(\lambda-\eta x)}{\pi^2(x^2+1)^2}\right]\\&=|\hat{\Lambda}|^{-1}\left[\frac{4\pi}{\eta}+2\pi^2ik+(2\pi)^3\sum_{\substack{\lambda\in\Lambda\\\lambda\ne0}}G_k(\lambda)e^{-i\theta\lambda}+o(1)\right]\quad\text{as }\eta\to0.\end{aligned}\tag{1.4.50}$$

Hence

$$\tilde{F}(\eta) = \int_0^\infty e^{-\eta\omega}\, d\left[f(\omega) - \frac{4\pi\omega}{|\hat{\Lambda}|}\right] = \frac{2\pi^2 ik}{|\hat{\Lambda}|} + \frac{(2\pi)^3}{|\hat{\Lambda}|} \sum_{\lambda\in\Lambda} \tilde{G}_k(\lambda) e^{-i\theta\lambda} + o(1) \quad (1.4.51)$$

implying

$$\begin{aligned}\lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\leq\omega}} \frac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - 4\pi\omega \right] &= |\hat{\Lambda}| \lim_{\omega\to\infty} \left[f(\omega) - \frac{4\pi\omega}{|\hat{\Lambda}|} \right] \\ &= |\hat{\Lambda}| \lim_{\eta\to 0} \tilde{F}(\eta) \\ &= (2\pi)^3 \left[\frac{ik}{4\pi} + \sum_{\lambda\in\Lambda} \tilde{G}_k(\lambda) e^{-i\theta\lambda} \right] \end{aligned} \quad (1.4.52)$$

which equals (1.4.47) when $a = 0$. Equation (1.4.47) for $a \in \mathbb{R}^3 - \Lambda$ follows in the same way except that now the term for $\lambda = 0$ needs no special treatment and the resulting series (over Γ) converges conditionally. ■

We now turn to the consistency problem mentioned at the beginning of this section, i.e., the proof that the operators $-\hat{\Delta}_{\alpha, Y+\Lambda}$ defined by (1.1.10) (with Y in (1.1.1) replaced by $Y + \Lambda$, where now Y is given by (1.4.27)) and $\int_{\hat{\Lambda}}^{\oplus} d^3\theta[-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)]$ are unitarily equivalent.

For completeness we will also prove the decomposition of the x-space version of $-\hat{\Delta}_{\alpha, Y+\Lambda}$, i.e., the operator $-\Delta_{\alpha, Y+\Lambda}$. Let

$$\begin{aligned} &\tilde{\mathscr{U}}: \mathscr{S}(\mathbb{R}^3) \to L^2(\hat{\Lambda}, |\hat{\Lambda}|^{-1}\, d^3\theta; L^2(\hat{\Gamma})) \equiv |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta\, L^2(\hat{\Gamma}), \\ &(\tilde{\mathscr{U}} f)(\theta, \nu) = \sum_{\lambda\in\Lambda} f(\nu + \lambda) e^{-i\theta\lambda}, \qquad \theta \in \hat{\Lambda}, \quad \nu \in \hat{\Gamma}, \quad f \in \mathscr{S}(\mathbb{R}^3), \end{aligned} \quad (1.4.53)$$

and extend $\tilde{\mathscr{U}}$ to all of $L^2(\mathbb{R}^3)$ by continuity (denoting the closure by the same symbol $\tilde{\mathscr{U}}$).

Theorem 1.4.3. *Let* $-\hat{\Delta}_{\alpha, Y+\Lambda}$ *be a self-adjoint operator defined by* (1.1.11) *where* $Y = \{y_1, \ldots, y_N\} \subset \hat{\Gamma}$ *and*

$$\alpha_j \equiv \alpha_{y_j+\lambda} \in \mathbb{R}, \qquad j = 1, \ldots, N, \quad \lambda \in \Lambda, \quad (1.4.54)$$

represents the strength of the δ*-interaction at the point* $y_j + \lambda \in Y + \Lambda$. *Then*

$$\mathscr{U}[-\hat{\Delta}_{\alpha, Y+\Lambda}]\mathscr{U}^{-1} = \int_{\hat{\Lambda}}^{\oplus} d^3\theta[-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)], \quad (1.4.55)$$

where $-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)$ *is given by* (1.4.34) *and* $\mathscr{U}$ *is given by* (1.4.16).

Furthermore, let $-\Delta_{\alpha, Y+\Lambda}$ *be defined by* (1.1.6) *with* Y *and* α *as above. Then*

$$\tilde{\mathscr{U}}[-\Delta_{\alpha, Y+\Lambda}]\tilde{\mathscr{U}}^{-1} = |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta[-\Delta_{\alpha,\Lambda,Y}(\theta)], \quad (1.4.56)$$

where $-\Delta_{\alpha,\Lambda,Y}(\theta)$ *is the self-adjoint operator in* $L^2(\hat{\Gamma})$ *with the resolvent*

$$(-\Delta_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}$$
$$= g_k(\theta) + |\hat{\Lambda}|^{-1} \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]_{jj'}^{-1} (\overline{g_k(\cdot - y_{j'}, \theta)}, \cdot) g_k(\cdot - y_j, \theta),$$
$$\det[\Gamma_{\alpha,\Lambda,Y}(k,\theta)] \neq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda},$$
$$\alpha_j \in \mathbb{R}, \quad y_j \in Y \subset \hat{\Gamma}, \quad j = 1, \ldots, N, \quad (1.4.57)$$

where

$$g_k(\theta): L^2(\hat{\Gamma}) \to L^2(\hat{\Gamma}),$$
$$(g_k(\theta)f)(v) = \int_{\hat{\Gamma}} d^3v'\, g_k(v - v', \theta) f(v'), \quad (1.4.58)$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \quad f \in L^2(\hat{\Gamma}),$$

and $g_k(v, \theta)$ *is given by* (1.4.37) (*or alternatively by* (1.4.38)).

PROOF. Using Theorem XIII.87 in [391] it is sufficient, for (1.4.5), to prove that

$$\mathscr{U}(-\hat{\Delta}_{\alpha,Y+\Lambda} - k^2)^{-1}\mathscr{U}^{-1} = \int_{\hat{\Lambda}}^{\oplus} d^3\theta (-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1} \quad (1.4.59)$$

for some $k^2 \in \mathbb{C} - \mathbb{R}$, $\operatorname{Im} k > 0$. By introducing the bounded operators

$$\tilde{A}_{\Lambda,Y}(k): L^2(\hat{\Lambda}, l^2(\Gamma)) \to \bigoplus_{j=1}^{N} l^2(\Lambda),$$
$$\Gamma_{\alpha,\Lambda,Y}(k): \bigoplus_{j=1}^{N} l^2(\Lambda) \to \bigoplus_{j=1}^{N} l^2(\Lambda), \quad (1.4.60)$$
$$\hat{B}_{\Lambda,Y}(k): \bigoplus_{j=1}^{N} l^2(\Lambda) \to L^2(\hat{\Lambda}, l^2(\Gamma)),$$

with

$$(\tilde{A}_{\Lambda,Y}(k)\mathscr{U}\hat{f})_j(\lambda) = (2\pi)^{-3/2} \int_{\hat{\Lambda}} d^3\theta \sum_{\gamma\in\Gamma} \frac{e^{i(\gamma+\theta)(y_j+\lambda)}}{|\gamma + \theta|^2 - k^2} \hat{f}(\gamma + \theta),$$
$$(\Gamma_{\alpha,\Lambda,Y}(k)a)_j(\lambda) = \sum_{j'=1}^{N} \sum_{\lambda'\in\Lambda} \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'}\delta_{\lambda\lambda'} - \tilde{G}_k(y_j - y_{j'} + \lambda - \lambda')\right] a_{j'}(\lambda'),$$
$$(\hat{B}_{\Lambda,Y}(k)a)(\theta, \gamma) = (2\pi)^{-3/2} \sum_{j=1}^{N} \sum_{\lambda\in\Lambda} \frac{e^{-i(\gamma+\theta)(y_j+\lambda)}}{|\gamma + \theta|^2 - k^2} a_j(\lambda),$$
$$k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k > 0, \quad \theta \in \hat{\Lambda}, \quad \hat{f} \in L^2(\mathbb{R}^3), \quad a \in \bigoplus_{j=1}^{N} l^2(\Lambda), \quad (1.4.61)$$

we observe after identifying $\bigoplus_{j=1}^{N} l^2(\Lambda)$ and $l^2(Y + \Lambda)$ that

$$(\hat{g}, (-\hat{\Delta}_{\alpha,Y+\Lambda} - k^2)^{-1}\hat{f}) = (\hat{g}, (p^2 - k^2)^{-1}\hat{f}) + (\mathscr{U}\hat{g}, \hat{B}_{\Lambda,Y}(k)[\Gamma_{\alpha,\Lambda,Y}(k)]^{-1}\tilde{A}_{\Lambda,Y}(k)\mathscr{U}\hat{f}),$$
$$k^2 \in \rho(-\hat{\Delta}_{\alpha,\Lambda,Y}), \quad \operatorname{Im} k > 0, \quad \hat{f}, \hat{g} \in L^2(\mathbb{R}^3), \quad (1.4.62)$$

where, in obvious notation, p denotes an integration variable. Furthermore, let $\mathscr{F}_\Lambda$ denote the Fourier transform, viz.

$$\begin{aligned}\mathscr{F}_\Lambda\colon & \bigoplus_{j=1}^{N} l^2(\Lambda) \to \bigoplus_{j=1}^{N} L^2(\hat{\Lambda}, |\hat{\Lambda}|^{-1}\, d^3\theta),\\ & (\mathscr{F}_\Lambda a)_j(\theta) = \sum_{\lambda\in\Lambda} a_j(\lambda) e^{-i\lambda\theta}, \qquad \theta\in\hat{\Lambda},\quad j=1,\ldots,N,\end{aligned} \tag{1.4.63}$$

$\mathscr{F}_\Lambda^{-1}$, its inverse, reads

$$\begin{aligned}\mathscr{F}_\Lambda^{-1}\colon & \bigoplus_{j=1}^{N} L^2(\hat{\Lambda}, |\hat{\Lambda}|^{-1}\, d^3\theta) \to \bigoplus_{j=1}^{N} l^2(\Lambda),\\ & (\mathscr{F}_\Lambda^{-1} f)_j(\lambda) = |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}} d^3\theta\, f_j(\theta) e^{i\lambda\theta}, \qquad \lambda\in\Lambda,\quad j=1,\ldots,N.\end{aligned} \tag{1.4.64}$$

Define

$$\begin{aligned}\tilde{A}_{\Lambda,Y}(k) &= \mathscr{F}_\Lambda \hat{A}_{\Lambda,Y}(k),\\ \tilde{\Gamma}_{\alpha,\Lambda,Y}(k) &= \mathscr{F}_\Lambda \Gamma_{\alpha,\Lambda,Y}(k)\mathscr{F}_\Lambda^{-1},\\ \tilde{B}_{\Lambda,Y}(k) &= \hat{B}_{\Lambda,Y}(k)\mathscr{F}_\Lambda^{-1}.\end{aligned} \tag{1.4.65}$$

$\Gamma_{\alpha,\Lambda,Y}(k)$, being a convolution operator in $\bigoplus_{j=1}^N l^2(\Lambda)$, transforms into a multiplication operator $\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta)$. In fact, we have

$$\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta) = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \sum_{\lambda\in\Lambda} \tilde{G}_k(y_j - y_{j'} + \lambda)e^{-i\lambda\theta}\right]_{j,j'=1}^{N},$$

$$\operatorname{Im} k > 0, \tag{1.4.66}$$

which can be seen as follows:

$$\begin{aligned}&(\mathscr{F}_\Lambda \Gamma_{\alpha,\Lambda,Y}(k)a)_j(\theta)\\ &\quad= \sum_{j'=1}^{N}\sum_{\lambda,\lambda'\in\Lambda}\left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'}\delta_{\lambda\lambda'} - \tilde{G}_k(y_j - y_{j'} + \lambda - \lambda')\right]e^{-i\theta(\lambda-\lambda')}e^{-i\lambda'\theta}a_{j'}(\lambda')\\ &\quad= (\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta))(\mathscr{F}_\Lambda a)(\theta))_j,\\ &\qquad\qquad \operatorname{Im} k>0,\quad \theta\in\hat{\Lambda},\quad j=1,\ldots,N,\quad a\in \textstyle\bigoplus_{j=1}^N l^2(\Lambda),\end{aligned} \tag{1.4.67}$$

where $\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta)$ is defined as above. Furthermore, we get by explicit computation that

$$\begin{aligned}(\tilde{B}_{\Lambda,Y}(k)f)(\theta,\gamma) &= \tilde{B}_{\Lambda,Y}(k,\theta,\gamma)f(\theta) = (2\pi)^{-3/2}\sum_{j=1}^{N}\frac{e^{-i(\gamma+\theta)y_j}}{|\gamma+\theta|^2 - k^2}f_j(\theta),\\ & k^2\notin|\Gamma+\theta|^2,\quad \operatorname{Im} k>0,\quad f=(f_1,\ldots,f_N)\in \textstyle\bigoplus_{j=1}^N L^2(\hat{\Lambda}),\end{aligned} \tag{1.4.68}$$

and

$$\begin{aligned}(\tilde{A}_{\Lambda,Y}(k)\mathscr{U}\hat{f})_j(\theta) &= (\tilde{A}_{\Lambda,Y}(k,\theta)\hat{f}(\theta+\cdot))_j = (2\pi)^{-3/2}|\hat{\Lambda}|\sum_{\gamma\in\Gamma}\frac{e^{i(\gamma+\theta)y_j}}{|\gamma+\theta|^2-k^2}\hat{f}(\gamma+\theta),\\ & k^2\notin|\Gamma+\theta|^2,\quad \operatorname{Im} k>0,\quad \hat{f}\in L^2(\mathbb{R}^3).\end{aligned} \tag{1.4.69}$$

Hence, using (1.4.62),

$$(\hat{g}, (-\hat{\Delta}_{\alpha,\Lambda+Y} - k^2)^{-1}\hat{f}) = \int_{\hat{\Lambda}}^{\oplus} d^3\theta\{((\mathscr{U}\hat{g})(\theta), G_k(\theta)(\mathscr{U}\hat{f})(\theta))_{l^2(\Gamma)}$$
$$+ ((\mathscr{U}\hat{g})(\theta), \tilde{B}_{\Lambda,Y}(k,\theta)[\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta)]^{-1}\tilde{A}_{\Lambda,Y}(k,\theta)(\mathscr{U}\hat{f})(\theta))_{l^2(\Gamma)}\},$$
$$k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \quad \hat{f}, \hat{g} \in L^2(\mathbb{R}^3). \quad (1.4.70)$$

But (1.4.70) is equivalent to

$$\mathscr{U}(-\hat{\Delta}_{\alpha,Y+\Lambda} - k^2)^{-1}\mathscr{U}^{-1} = \int_{\hat{\Lambda}}^{\oplus} d^3\theta[G_k(\theta) + \tilde{B}_{\Lambda,Y}(k,\theta)[\tilde{\Gamma}_{\alpha,\Lambda,Y}(k,\theta)]^{-1}\tilde{A}_{\Lambda,Y}(k,\theta)],$$
$$k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \quad (1.4.71)$$

and by appealing to Lemma 1.4.2 we see that the integrand on the right-hand side exactly equals $(-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}$, proving (1.4.55). To prove (1.4.56) we could decompose the resolvent directly as in the proof of (1.4.54), or alternatively combine (1.4.54) and the unitary equivalence of $-\Delta_{\alpha,Y+\Lambda}$ and $-\hat{\Delta}_{\alpha,Y+\Lambda}$. Here we will follow the latter approach. Thus

$$\begin{aligned}
&(g, (-\Delta_{\alpha,Y+\Lambda} - k^2)^{-1}f) \\
&\quad = (\mathscr{F}g, (-\hat{\Delta}_{\alpha,Y+\Lambda} - k^2)^{-1}\mathscr{F}f) \\
&\quad = \left(\mathscr{U}\mathscr{F}g, \int_{\hat{\Lambda}}^{\oplus} d^3\theta(-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}\mathscr{U}\mathscr{F}f\right) \\
&\quad = \left(\mathscr{U}\mathscr{F}g, \int_{\hat{\Lambda}}^{\oplus} d^3\theta\, G_k(\theta)\mathscr{U}\mathscr{F}f\right) \\
&\qquad + \sum_{j,j'=1}^{N} \int_{\hat{\Lambda}} d^3\theta[\Gamma_{\alpha,\Lambda,Y}(k,\theta)]_{jj'}^{-1}(\mathscr{U}\mathscr{F}g, F_{k,y_j}(\theta))(F_{-\bar{k},y_j}(\theta), \mathscr{U}\mathscr{F}f) \\
&\quad = \int_{\hat{\Lambda}} d^3\theta\Big\{(\bar{\mathscr{F}}_\Gamma(\theta)(\mathscr{U}\mathscr{F}g)(\theta), \bar{\mathscr{F}}_\Gamma(\theta)G_k^{-1}(\theta)\bar{\mathscr{F}}_\Gamma^{-1}(\theta)\bar{\mathscr{F}}_\Gamma(\theta)(\mathscr{U}\mathscr{F}f)(\theta)) \\
&\qquad + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]_{jj'}^{-1}(\bar{\mathscr{F}}_\Gamma(\theta)(\mathscr{U}\mathscr{F}g)(\theta), \\
&\qquad \bar{\mathscr{F}}_\Gamma(\theta)F_{k,y_j}(\theta))(\bar{\mathscr{F}}_\Gamma(\theta)F_{-\bar{k},y_{j'}}(\theta), \bar{\mathscr{F}}_\Gamma(\theta)(\mathscr{U}\mathscr{F}f)(\theta))\Big\} \\
&\quad = |\hat{\Lambda}|^{-1}\int_{\hat{\Lambda}} d^3\theta\Big\{((\tilde{\mathscr{U}}g)(\theta), g_k(\theta)(\tilde{\mathscr{U}}f)(\theta)) \\
&\qquad + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda,Y}(k,\theta)]_{jj'}^{-1}((\tilde{\mathscr{U}}g)(\theta), g_k(\cdot - y_j,\theta))(\overline{g_k(\cdot - y_{j'},\theta)}, (\mathscr{U}f)(\theta))\Big\} \\
&\quad = \left(\tilde{\mathscr{U}}g, |\hat{\Lambda}|^{-1}\int_{\hat{\Lambda}}^{\oplus} d^3\theta(-\Delta_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}\tilde{\mathscr{U}}f\right),
\end{aligned}$$
$$f, g \in L^2(\mathbb{R}^3), \quad (1.4.72)$$

where $\bar{\mathscr{F}}_\Gamma(\theta)$ is the Fourier transform

$$\bar{\mathscr{F}}_\Gamma(\theta): l^2(\Gamma) \to L^2(\hat{\Gamma}),$$
$$(\bar{\mathscr{F}}_\Gamma(\theta)a)(v) = |\hat{\Gamma}|^{-1/2} e^{i\theta v} \sum_{\gamma \in \Gamma} a_\gamma e^{i\gamma v}, \qquad \theta \in \hat{\Lambda}, \quad v \in \hat{\Gamma}, \quad a \in l^2(\Gamma). \tag{1.4.73}$$

■

Remark. $g_k(\theta)$ is, of course, the resolvent of the decomposed Laplacian $-\Delta(\theta)$, i.e.,

$$g_k(\theta) = (-\Delta(\theta) - k^2)^{-1}, \qquad k^2 \in \rho(-\Delta(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \tag{1.4.74}$$

where $-\Delta(\theta)$ is the self-adjoint operator $-(\partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2)$ on $L^2(\hat{\Gamma})$ with boundary conditions

$$f(v + a_j) = e^{i\theta a_j} f(v), \qquad \frac{\partial f}{\partial x_j}(v + a_j) = e^{i\theta a_j} \frac{\partial f}{\partial x_j}(v),$$
$$\theta = (\theta_1, \theta_2, \theta_3) \in \hat{\Lambda}, \quad v, v + a_j \in \partial\hat{\Gamma}, \quad j = 1, 2, 3. \tag{1.4.75}$$

Having settled the consistency question we now turn to the detailed study of spectral properties of the operators $-\hat{\Delta}_{\alpha, Y+\Lambda}$ and $-\hat{\Delta}_{\alpha, Y, \Lambda}(\theta)$. First, we consider the case where Y consists of one point which, by translation invariance, can be assumed to be zero, i.e., $Y = \{0\}$. We then write $-\hat{\Delta}_{\alpha,\Lambda}$ and $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ for $-\hat{\Delta}_{\alpha,\{0\}+\Lambda}$ and $-\hat{\Delta}_{\alpha,\Lambda,\{0\}}(\theta)$, respectively, and we use α instead of α_0. We can now state the following

Theorem 1.4.4. *The spectrum of* $-\hat{\Delta}_{\alpha,\Lambda}(\theta) \equiv -\hat{\Delta}_{\alpha,\Lambda,\{0\}}(\theta)$, $\alpha \in \mathbb{R}$, *is purely discrete and consists of isolated eigenvalues of finite multiplicity for all* $\theta \in \hat{\Lambda}$, *i.e.,*

$$\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda}(\theta)) = \varnothing, \qquad \theta \in \hat{\Lambda}. \tag{1.4.76}$$

More precisely, it can be characterized as follows: $\mathbb{R} - |\Gamma + \theta|^2$ *consists of an infinite union of disjoint open intervals* $I_n(\theta)$, *i.e.,*

$$\mathbb{R} - |\Gamma + \theta|^2 = \bigcup_{n=0}^{\infty} I_n(\theta). \tag{1.4.77}$$

Here $I_0 = (-\infty, \theta^2)$ *and* $I_n(\theta)$, $n \in \mathbb{N}$, *are bounded intervals. In each interval,* $I_n(\theta)$, $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ *has exactly one simple eigenvalue* $E_n^{\alpha,\Lambda}(\theta)$ *with eigenfunction*

$$\psi_{E_n^{\alpha,\Lambda}(\theta)}(\gamma) = [|\gamma + \theta|^2 - E_n^{\alpha,\Lambda}(\theta)]^{-1}, \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma. \tag{1.4.78}$$

Furthermore, $E_n^{\alpha,\Lambda}(\theta)$ *is strictly increasing in* α *for* $n \in \mathbb{N}$, $\theta \in \hat{\Lambda}$. *In addition,* $E^\Lambda(\theta) \in |\Gamma + \theta|^2$ *is an eigenvalue of* $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ *of multiplicity* $m \geq 1$ *iff there exist* $m + 1$ *points* $\gamma_0, \ldots, \gamma_m \in \Gamma$ *such that*

$$E^\Lambda(\theta) = |\gamma_0 + \theta|^2 = \cdots = |\gamma_m + \theta|^2. \tag{1.4.79}$$

The corresponding eigenspace is spanned by the eigenfunctions

$$\psi_{E^\Lambda(\theta)}^{(j)}(\gamma) = \delta_{\gamma\gamma_j} - \delta_{\gamma\gamma_0}, \qquad \theta \in \hat{\Lambda}, \quad \gamma, \gamma_j \in \Gamma, \quad j = 1, \ldots, m, \tag{1.4.80}$$

$-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ *has no other eigenvalues.*

PROOF. Recall that the unperturbed operator $-\hat{\Delta}(\theta)$ has a purely discrete spectrum with eigenvalues $|\gamma + \theta|^2$, $\gamma \in \Gamma$ (cf. (1.4.23)), i.e., $\sigma(-\hat{\Delta}(\theta)) = |\Gamma + \theta|^2$. From the explicit expression (1.4.34) we see that there are two possibilities for eigenvalues of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$, namely

(a) $\alpha = g_{E^{1/2}}(0, \theta)$,
(b) $E(\theta) = |\gamma + \theta|^2$.

For case (a) we observe the following properties of the function $g_k(0, \theta)$ as a function of k^2:

(i) The poles of $g_k(0, \theta)$ are exactly the elements of $|\Gamma + \theta|^2$.

(ii) $\dfrac{\partial g_k(0, \theta)}{\partial(k^2)} = |\hat{\Gamma}|^{-1} \sum_{\gamma \in \Gamma} \dfrac{1}{(|\gamma + \theta|^2 - k^2)^2} > 0, \qquad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0.$

(iii) $g_k(0, \theta) \to -\infty \quad$ as $k^2 \to -\infty$.

Thus we obtain the graph of $g_k(0, \theta)$ as in Figure 5, and writing

$$\mathbb{R} - |\Gamma + \theta|^2 = \bigcup_{n=0}^{\infty} I_n(\theta), \qquad \theta \in \hat{\Lambda}, \tag{1.4.81}$$

where $I_0(\theta) = (-\infty, |\theta|^2)$ is the unique unbounded interval, we see that there is exactly one eigenvalue $E_n^{\alpha,\Lambda}(\theta)$ of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ in each interval $I_n(\theta)$, and this eigenvalue is in case (a). To find the corresponding eigenfunction and multiplicity we use ([283], p. 180)

$$\operatorname*{n-lim}_{z \to E} (E - z)(H - z)^{-1} = P \tag{1.4.82}$$

for self-adjoint operators H, when E is an isolated point of the spectrum of H,

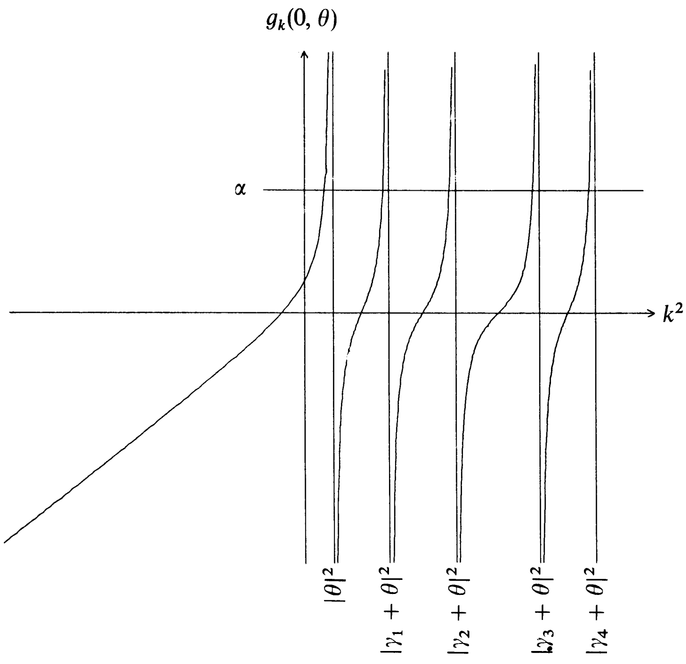


Figure 5 Qualitative behavior of $g_k(0, \theta)$ as a function of k^2.

and P is the projection onto the eigenspace belonging to the eigenvalue E. Using the explicit form of the resolvent we get

$$\begin{aligned} P_n^{\alpha,\Lambda}(\theta) &= \underset{z \to E_n^{\alpha,\Lambda}(\theta)}{\text{n-lim}} (E_n^{\alpha,\Lambda}(\theta) - z)(-\hat{\Delta}_{\alpha,\Lambda}(\theta) - z)^{-1} \\ &= \|\psi_{E_n^{\alpha,\Lambda}(\theta)}\|^{-2}(\psi_{E_n^{\alpha,\Lambda}(\theta)}, \cdot)\psi_{E_n^{\alpha,\Lambda}(\theta)}, \qquad n \in \mathbb{N}_0, \end{aligned} \tag{1.4.83}$$

where $\psi_{E_n^{\alpha,\Lambda}(\theta)}$ is given by (1.4.78) and $\|\cdot\|$ denotes the norm in $l^2(\Gamma)$.

In case (b) a more detailed analysis is required since $E^\Lambda(\theta) = |\gamma + \theta|^2$ is a singularity in all terms of the resolvent. Assume that there are $m + 1$ points $\gamma_0, \ldots, \gamma_m \in \Gamma$ such that

$$E^\Lambda(\theta) = |\gamma_0 + \theta|^2 = \cdots = |\gamma_m + \theta|^2. \tag{1.4.84}$$

First, we observe that, as $k^2 \to E^\Lambda(\theta)$,

$$|\hat{\Gamma}|[\alpha - g_k(0, \theta)]^{-1} = -(m + 1)^{-1}(E^\Lambda(\theta) - k^2) + o(k^2 - E^\Lambda(\theta))$$

because there are exactly $m + 1$ points, each of which gives rise to a simple pole of $g_k(0, \theta)$ with residuum $|\hat{\Gamma}|^{-1}$. Furthermore, we decompose the function $(|\gamma + \theta|^2 - k^2)^{-1}$ as follows

$$(|\gamma + \theta|^2 - k^2)^{-1} = \Phi_{1,k}(\gamma) + \Phi_{2,k}(\gamma), \qquad \gamma \in \Gamma, \quad \theta \in \hat{\Lambda}, \tag{1.4.85}$$

where

$$\begin{aligned} \Phi_{1,k}(\gamma) &= \chi_{\{\gamma_0, \ldots, \gamma_m\}}(\gamma)(|\gamma + \theta|^2 - k^2)^{-1}, \\ \Phi_{2,k}(\gamma) &= (1 - \chi_{\{\gamma_0, \ldots, \gamma_m\}}(\gamma))(|\gamma + \theta|^2 - k^2)^{-1}, \qquad \gamma \in \Gamma, \quad \theta \in \hat{\Lambda}. \end{aligned} \tag{1.4.86}$$

Here χ_A denotes the characteristic function of a subset $A \subseteq \Gamma$. Then $(-\hat{\Delta}_{\alpha,\Lambda}(\theta) - k^2)^{-1}$ takes the form

$$\begin{aligned} (-\hat{\Delta}_{\alpha,\Lambda}(\theta) - k^2)^{-1} = \Phi_{1,k} &+ \Phi_{2,k} - (m + 1)^{-1}(E^\Lambda(\theta) - k^2)(\Phi_{1,k}, \cdot)\Phi_{1,k} \\ &+ [-(m + 1)^{-1}(E^\Lambda(\theta) - k^2) + o(E^\Lambda(\theta) - k^2)] \cdot \\ &\cdot [(\Phi_{1,k}, \cdot)\Phi_{2,k} + (\Phi_{2,k}, \cdot)\Phi_{1,k} + (\Phi_{2,k}, \cdot)\Phi_{2,k}] \\ &+ o(E^\Lambda(\theta) - k^2)(\Phi_{1,k}, \cdot)\Phi_{1,k}, \end{aligned} \tag{1.4.87}$$

and hence

$$\begin{aligned} P^\Lambda(\theta) &= \underset{k^2 \to E^\Lambda(\theta)}{\text{n-lim}} (E^\Lambda(\theta) - k^2)(-\hat{\Delta}_{\alpha,\Lambda}(\theta) - k^2)^{-1} \\ &= \begin{cases} \chi_{\{\gamma_0, \ldots, \gamma_m\}} - (m + 1)^{-1}(\chi_{\{\gamma_0, \ldots, \gamma_m\}}, \cdot)\chi_{\{\gamma_0, \ldots, \gamma_m\}}, & m \geq 1, \\ 0, \quad m = 0, \end{cases} \end{aligned} \tag{1.4.88}$$

since

$$(E^\Lambda(\theta) - k^2)\Phi_{1,k} - \chi_{\{\gamma_0, \ldots, \gamma_m\}} \xrightarrow[k^2 \to E^\Lambda(\theta)]{n} 0 \tag{1.4.89}$$

as a multiplication operator, and

$$(E^\Lambda(\theta) - k^2)((E^\Lambda(\theta) - k^2)\Phi_{1,k}, \cdot)\Phi_{1,k} \xrightarrow[k^2 \to E^\Lambda(\theta)]{n} (\chi_{\{\gamma_0, \ldots, \gamma_m\}}, \cdot)\chi_{\{\gamma_0, \ldots, \gamma_m\}}. \tag{1.4.90}$$

In particular, if $m = 0$, then $P^\Lambda(\theta) = 0$, i.e., there is no eigenvalue. Now, assume that $m \geq 1$, and define

$$\begin{aligned} \psi_j(\gamma) &= \delta_{\gamma\gamma_j} - \delta_{\gamma\gamma_0}, \qquad j = 1, \ldots, m, \\ \phi_j(\gamma) &= \delta_{\gamma\gamma_j} - (m + 1)^{-1} \sum_{j'=0}^{m} \delta_{\gamma\gamma_{j'}}, \qquad j = 0, \ldots, m. \end{aligned} \tag{1.4.91}$$

Then

$$\phi_0 = -\sum_{j=1}^{m} \phi_j \tag{1.4.92}$$

and hence $P^\Lambda(\theta)$ can be written

$$\begin{aligned}(P^\Lambda(\theta)f)(\gamma) &= \sum_{j=0}^{m} \delta_{\gamma\gamma_j} f(\gamma_j) - (m+1)^{-1}[f(\gamma_0) + \cdots + f(\gamma_m)] \sum_{j=0}^{m} \delta_{\gamma\gamma_j} \\ &= \sum_{j=0}^{m} \delta_{\gamma\gamma_j}\{f(\gamma_j) - (m+1)^{-1}[f(\gamma_0) + \cdots + f(\gamma_m)]\} \\ &= \sum_{j=0}^{m} \delta_{\gamma\gamma_j}(\phi_j, f) = \sum_{j=0}^{m} (\delta_{\gamma\gamma_j} - \delta_{\gamma\gamma_0})(\phi_j, f) \\ &= \sum_{j=1}^{m} (\phi_j, f)\psi_j(\gamma), \qquad \gamma \in \Gamma, \quad f \in l^2(\Gamma),\end{aligned} \tag{1.4.93}$$

which proves that $\dim P^\Lambda = m$ and that $\psi_1, \ldots, \psi_m$ span the corresponding eigenspace. ■

Remarks. 1. The above proof shows that there is a natural one-to-one correspondence $\Gamma \to \sigma(-\hat{\Delta}_{\alpha,\Lambda}(\theta))$ in the following sense, when $\sigma(-\hat{\Delta}_{\alpha,\Lambda}(\theta))$ is considered with multiplicities: Namely, let $\gamma \in \Gamma$. If $|\gamma + \theta|^2$ is no eigenvalue, we define $E_\gamma^{\alpha,\Lambda}(\theta)$ to be the largest eigenvalue of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ smaller than $|\gamma + \theta|^2$. (This will necessarily be an eigenvalue in case (a), i.e., a solution of $\alpha = g_{E^{1/2}}(0, \theta)$.) If $|\gamma + \theta|^2$ is an eigenvalue with multiplicity m, then there exist $m + 1$ points $\gamma = \gamma_0, \gamma_1, \ldots, \gamma_m \in \Gamma$ such that $|\gamma_0 + \theta|^2 = \cdots = |\gamma_m + \theta|^2$ and we let $E_{\gamma_{j_0}}^{\alpha,\Lambda}(\theta)$ be as above for one $j_0 \in \{0, \ldots, m\}$, and $E_{\gamma_j}^{\Lambda}(\theta) = |\gamma + \theta|^2$ for all $j \neq j_0$. Henceforth we will use this correspondence.

2. We remark that for the lowest eigenvalue one is always in case (a).

Using the properties of the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ we will now study the spectrum of the full Hamiltonian $-\hat{\Delta}_{\alpha,\Lambda}$.

Theorem 1.4.5. *Let Λ be a lattice in the sense of* (1.4.3) *and let $\alpha \in \mathbb{R}$. Then the spectrum of the operator*

$$-\hat{\Delta}_{\alpha,\Lambda} = \mathscr{U}^{-1}\left\{\int_{\hat{\Lambda}}^{\oplus} d^3\theta\,[-\hat{\Delta}_{\alpha,\Lambda}(\theta)]\right\}\mathscr{U} \tag{1.4.94}$$

is purely absolutely continuous and equals

$$\begin{aligned}&\sigma(-\hat{\Delta}_{\alpha,\Lambda}) = \sigma_{\rm ac}(-\hat{\Delta}_{\alpha,\Lambda}) = [E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)] \cup [E_1^{\alpha,\Lambda}, \infty), \\ &\sigma_{\rm sc}(-\hat{\Delta}_{\alpha,\Lambda}) = \varnothing, \qquad \alpha \in \mathbb{R},\end{aligned} \tag{1.4.95}$$

where

$$\theta_0 = -\tfrac{1}{2}(b_1 + b_2 + b_3) \tag{1.4.96}$$

and

$$E_1^{\alpha,\Lambda} = \min\{E_{b_-}^{\alpha,\Lambda}(0), \tfrac{1}{4}|b_-|^2\} = \min_{\theta \in \hat{\Lambda}}[E_{b_-}^{\alpha,\Lambda}(\theta)], \tag{1.4.97}$$

where $b_- \in \{b_1, b_2, b_3\}$ is such that

$$|b_-| \leq |b_j|, \qquad j = 1, 2, 3. \tag{1.4.98}$$

We have that

$$E_1^{\alpha,\Lambda} > 0, \qquad \alpha \in \mathbb{R}, \tag{1.4.99}$$

and

$$E_0^{\alpha,\Lambda}(\theta_0) < 0 \quad \textit{iff} \quad \alpha < \alpha_{0,\Lambda} \tag{1.4.100}$$

with

$$\alpha_{0,\Lambda} = g_0(0, \theta_0). \tag{1.4.101}$$

Furthermore, the spectrum is monotone increasing in α in the sense that

$$\frac{\partial E_\gamma^{\alpha,\Lambda}(\theta)}{\partial \alpha} > 0, \qquad \gamma \in \Gamma, \quad \theta \in \hat{\Lambda}, \qquad \frac{\partial E_1^{\alpha,\Lambda}}{\partial \alpha} \geq 0. \tag{1.4.102}$$

In addition,

$$E_0^{\alpha,\Lambda}(0) \to \begin{cases} 0, & \alpha \to \infty, \\ -\infty, & \alpha \to -\infty, \end{cases} \qquad E_0^{\alpha,\Lambda}(\theta_0) \to \begin{cases} |\theta_0|^2, & \alpha \to \infty, \\ -\infty, & \alpha \to -\infty, \end{cases}$$
$$E_1^{\alpha,\Lambda} \to \begin{cases} \frac{1}{4}|b_-|^2, & \alpha \to \infty, \\ 0, & \alpha \to -\infty, \end{cases} \tag{1.4.103}$$

and hence there exists an $\alpha_{1,\Lambda} \in \mathbb{R}$ such that

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda}) = [E_0^{\alpha,\Lambda}(0), \infty), \qquad \alpha \geq \alpha_{1,\Lambda}. \tag{1.4.104}$$

PROOF. We now have to study in detail the behavior in $\theta \in \hat{\Lambda}$ of the eigenvalues $E_\gamma^{\alpha,\Lambda}(\theta)$ of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$. (We use the labeling of the eigenvalues introduced in the first remark after the preceding theorem.) The lowest band comes from the eigenvalue $E_0^{\alpha,\Lambda}(\theta)$, i.e., with $\gamma = 0$. As remarked earlier, this eigenvalue is in case (a), i.e., a solution of

$$\alpha = g_{E^{1/2}}(0, \theta), \qquad \operatorname{Im} E^{1/2} \geq 0. \tag{1.4.105}$$

To simplify the notation in this part of the proof we assume that $\Lambda = \mathbb{Z}^3$, thus $\Gamma = 2\pi\mathbb{Z}^3$ and $\hat{\Lambda} = [-\pi, \pi)^3$. From (1.4.105) we infer (where ∇ denotes the gradient with respect to θ)

$$\nabla g_{\sqrt{E_0^{\alpha,\Lambda}(\theta)}}(0, \theta) + \left.\frac{\partial g_{E^{1/2}}(0, \theta)}{\partial E}\right|_{E = E_0^{\alpha,\Lambda}(\theta)} \nabla E_0^{\alpha,\Lambda}(\theta) = 0, \tag{1.4.106}$$

which implies that the stationary points of $g_{E^{1/2}}(0, \theta)$ and $E_0^{\alpha,\Lambda}(\theta)$ (with respect to θ) coincide. We have

$$\nabla g_{E^{1/2}}(0, \theta) = -(2\pi)^{-3} \lim_{\omega \to \infty} \sum_{\substack{\gamma \in \Gamma \\ |\gamma + \theta| \leq \omega}} \frac{2(\gamma + \theta)}{(|\gamma + \theta|^2 - E)^2}, \tag{1.4.107}$$

and by considering the first component $(\nabla g_{E^{1/2}})^1(0, \theta)$ of $\nabla g_{E^{1/2}}(0, \theta)$ and summing the series (1.4.107) in this component we find

$$(\nabla g_{E^{1/2}})^1(0, \theta) = -\frac{1}{64\pi^4} \sum_{\tilde{\gamma} \in 2\pi\mathbb{Z}^2} \frac{\sin[2\pi B_{\tilde{\gamma}}(E, \tilde{\theta})] \sin \theta_1}{B_{\tilde{\gamma}}(E, \tilde{\theta})\{\cos[2\pi B_{\tilde{\gamma}}(E, \tilde{\theta})] - \cos \theta_1\}^2},$$
$$\theta = (\theta_1, \theta_2, \theta_3), \quad \tilde{\theta} = (0, \theta_2, \theta_3), \quad B_{\tilde{\gamma}}(E, \tilde{\theta}) = \sqrt{E - (\tilde{\gamma} + \tilde{\theta})^2},$$
$$\operatorname{Im} B_{\tilde{\gamma}}(E, \tilde{\theta}) \geq 0, \quad \tilde{\gamma} \in 2\pi\mathbb{Z}^2. \quad (1.4.108)$$

Since

$$\frac{\sin[2\pi B_{\tilde{\gamma}}(E, \tilde{\theta})]}{B_{\tilde{\gamma}}(E, \tilde{\theta})} > 0 \quad (1.4.109)$$

as long as $E < |\tilde{\theta}|^2 + \frac{1}{4}$, we see that

$$\nabla g_{E^{1/2}}(0, \theta) = 0 \quad \textit{iff} \quad \theta \in \{0, -\tfrac{1}{2}(b_1 + b_2 + b_3)\}. \quad (1.4.110)$$

Furthermore, we have that $\theta = 0$ gives a minimum and $\theta = \theta_0$ gives a maximum, thus

$$E_0^{\alpha,\Lambda}(0) \leq E_0^{\alpha,\Lambda}(\theta) \leq E_0^{\alpha,\Lambda}(\theta_0). \quad (1.4.111)$$

Let $E_1^{\alpha,\Lambda}$ denote the bottom of the second band, i.e.,

$$E_1^{\alpha,\Lambda} = \min_{\theta \in \hat{\Lambda}} [E_{b_-}^{\alpha,\Lambda}(\theta)]. \quad (1.4.112)$$

From Theorem 1.4.4 we have

$$|\theta|^2 \leq E_{b_-}^{\alpha,\Lambda}(\theta) \leq (b_- + \theta)^2 \quad (1.4.113)$$

and hence

$$E_{b_-}(-\tfrac{1}{2}b_-) = \tfrac{1}{4}|b_-|^2. \quad (1.4.114)$$

If $E_1^{\alpha,\Lambda} < \frac{1}{4}|b_-|^2$, then the above argument shows that $E_1^{\alpha,\Lambda} = E_{b_-}^{\alpha,\Lambda}(0)$. To prove that there are no gaps in the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}$ above $E_1^{\alpha,\Lambda}$ we first extend $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ to all $\theta \in \mathbb{R}^3$ by using the same expression (1.4.34) (with $N = 1$, $y_1 = 0$, $\alpha_1 = \alpha$) for the resolvent. Due to the periodicity we have

$$\bigcup_{\theta \in \hat{\Lambda}} \sigma(-\hat{\Delta}_{\alpha,\Lambda}(\theta)) = \bigcup_{\theta \in \mathbb{R}^3} \sigma(-\hat{\Delta}_{\alpha,\Lambda}(\theta)). \quad (1.4.115)$$

The definition of $E_\gamma^{\alpha,\Lambda}(\theta)$ for $\theta \in \hat{\Lambda}$, $\gamma \in \Gamma$, can be extended continuously to all $\theta \in \mathbb{R}^3$ by the same procedure. Using (1.4.102), and the continuity of $E_\gamma^{\alpha,\Lambda}(\theta)$ for $\theta \in \mathbb{R}^3$, we infer ([391], Theorem XIII.85)

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda}) = \bigcup_{\theta \in \hat{\Lambda}} \sigma(-\hat{\Delta}_{\alpha,\Lambda}(\theta)) = \{E_\gamma^{\alpha,\Lambda}(\theta) | \theta \in \mathbb{R}^3, \gamma \in \Gamma\}. \quad (1.4.116)$$

Assume now that there is a gap in the positive part of the spectrum, say $[a, b] \subseteq \rho(-\hat{\Delta}_{\alpha,\Lambda})$, $b > a > E_1^{\alpha,\Lambda}$. Then we can find $\gamma, \gamma', \gamma'' \in \Gamma$, not on a line, and $\bar{\theta} \in \mathbb{R}^3$ such that

$$|\gamma'' + \bar{\theta}|^2 < E_\gamma^{\alpha,\Lambda}(\bar{\theta}) < a < b < E_{\gamma'}^{\alpha,\Lambda}(\bar{\theta}) < |\gamma' + \bar{\theta}|^2. \quad (1.4.117)$$

We may assume that

$$|\gamma'' + \theta|^2 \leq E_\gamma^{\alpha,\Lambda}(\theta) \leq |\gamma + \theta|^2 \leq E_{\gamma'}^{\alpha,\Lambda}(\theta) \leq |\gamma' + \theta|^2, \qquad \theta \in \mathbb{R}^3, \quad (1.4.118)$$

as long as

$$|\gamma'' + \theta|^2 \le |\gamma + \theta|^2 \le |\gamma' + \theta|^2, \qquad \theta \in \mathbb{R}^3. \tag{1.4.119}$$

However, we can always find a $\tilde{\theta} \in \mathbb{R}^3$ such that

$$|\gamma'' + \tilde{\theta}| = |\gamma' + \tilde{\theta}| = |\gamma + \tilde{\theta}|. \tag{1.4.120}$$

For this $\tilde{\theta}$ we have

$$E_{\gamma}^{\alpha,\Lambda}(\tilde{\theta}) = E_{\gamma'}^{\alpha,\Lambda}(\tilde{\theta}) \tag{1.4.121}$$

and hence, $E_{\gamma}^{\alpha,\Lambda}(\theta)$ being continuous,

$$[a, b] \subset [E_{\gamma}^{\alpha,\Lambda}(\bar{\theta}), E_{\gamma'}^{\alpha,\Lambda}(\bar{\theta})] \subseteq \sigma(-\hat{\Delta}_{\alpha,\Lambda}), \tag{1.4.122}$$

which yields a contradiction to the assumption that there was a gap in the positive part of the spectrum. The absolute continuity of the spectrum follows from Lemmas 10.14 and 10.15 in [85]. The monotonicity in α of $E_{\gamma}^{\alpha,\Lambda}(\theta)$ follows by differentiating (1.4.105) with respect to α. ∎

In the general case, where Y consists of N points, we do not have that detailed information on the spectrum of $-\hat{\Delta}_{\alpha,Y+\Lambda}$, except for the fact that the negative part of the spectrum consists of at most N bands, which is the content of the next theorem.

Theorem 1.4.6. *Let $\alpha_j \in \mathbb{R}$, $y_j \in Y$, $j = 1, \ldots, N$. Then $\sigma(-\hat{\Delta}_{\alpha,Y+\Lambda}) \cap (-\infty, 0)$ consists of at most N disjoint, closed intervals where*

$$\mathscr{U}[-\hat{\Delta}_{\alpha,Y+\Lambda}]\mathscr{U}^{-1} \equiv \int_{\hat{\Lambda}}^{\oplus} d^3\theta[-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)]. \tag{1.4.123}$$

Proof. As in the proof of Theorem II.1.1.4 we will first prove that $\Gamma_{\alpha,\Lambda,Y}(k,\theta)$ is monotone decreasing in k^2 for $k^2 < 0$. It is equivalent to proving the same property for $\mathscr{U}_\theta\Gamma_{\alpha,\Lambda,Y}(k,\theta)\mathscr{U}_\theta^{-1}$ where $\mathscr{U}_x$ is the unitary operator

$$\mathscr{U}_x\colon \mathbb{C}^N \to \mathbb{C}^N, \qquad (\mathscr{U}_x a)_j = e^{-ixy_j}a_j, \qquad j = 1, \ldots, N, \quad a = (a_1, \ldots, a_N) \in \mathbb{C}^N,$$
$$x \in \mathbb{R}^3. \tag{1.4.124}$$

We have

$$(a, \mathscr{U}_\theta\Gamma_{\alpha,\Lambda,Y}(k,\theta)\mathscr{U}_\theta^{-1}a)$$
$$= \sum_{j=1}^N \alpha_j|a_j|^2 - (2\pi)^{-3}\lim_{\omega\to\infty}\left[\sum_{\substack{\gamma\in\Gamma\\|\gamma+\theta|\le\omega}} \frac{|\hat{\Lambda}|\left|\sum_{j=1}^N (\mathscr{U}_\gamma a)_j\right|^2}{|\gamma+\theta|^2 - k^2} - 4\pi\omega\sum_{j=1}^N |a_j|^2\right] \tag{1.4.125}$$

which proves the monotonicity in k^2, $k^2 < 0$. Hence $\Gamma_{\alpha,\Lambda,Y}(k,\theta)$ has at most N eigenvalues which are all strictly decreasing and each of which can give rise to at most one band in the negative part of the spectrum of $-\hat{\Delta}_{\alpha,Y+\Lambda}$. ∎

We will now study how $-\Delta_{\alpha,Y+\Lambda}$ can be approximated by scaled short-range Hamiltonians. The general Theorem 1.2.1 covers this situation. However, to obtain detailed properties of the behavior of the spectrum, we have to study the decomposed operator $-\hat{\Delta}_{\alpha,\Lambda,Y}(\theta)$. We start by decomposing the operator $H_{\varepsilon,Y+\Lambda}$.

Theorem 1.4.7. *Let $V_j \in R$, supp V_j compact, be real-valued and let $\lambda_j(\varepsilon) = 1 + \varepsilon\lambda_j'(0) + o(\varepsilon)$ as $\varepsilon \downarrow 0, j = 1, \ldots, N$. Then the self-adjoint operator*

$$H_{\varepsilon,Y+\Lambda} = -\Delta \dotplus \varepsilon^{-2} \sum_{j=1}^{N} \sum_{\lambda\in\Lambda} \lambda_j(\varepsilon) V_j((\cdot - y_j - \lambda)/\varepsilon) \tag{1.4.126}$$

in $L^2(\mathbb{R}^3)$ can be decomposed

$$\tilde{\mathcal{U}} H_{\varepsilon,Y+\Lambda} \tilde{\mathcal{U}}^{-1} = |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, H_{\varepsilon,\Lambda,Y}(\theta), \tag{1.4.127}$$

where $H_{\varepsilon,\Lambda,Y}(\theta)$ is the self-adjoint operator in $L^2(\hat{\Gamma})$ with the resolvent

$$(H_{\varepsilon,\Lambda,Y}(\theta) - k^2)^{-1} = g_k(\theta) - \varepsilon \sum_{j,j'=1}^{N} A_{\varepsilon,j}(k,\theta)[1 + B_\varepsilon(k,\theta)]_{jj'}^{-1} C_{\varepsilon,j'}(k,\theta),$$

$$k^2 \in \rho(H_{\varepsilon,\Lambda,Y}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}. \tag{1.4.128}$$

Here $g_k(\theta)$ is given by (1.4.58), while the Hilbert–Schmidt operators $A_{\varepsilon,j}(k,\theta)$, $B_\varepsilon(k,\theta)$, and $C_{\varepsilon,j}(k,\theta)$ are defined by

$$\begin{aligned} &A_{\varepsilon,j}(k,\theta)\colon L^2(\mathbb{R}^3) \to L^2(\hat{\Gamma}), \\ &B_\varepsilon(k,\theta) = [B_{\varepsilon,jj'}(k,\theta)]_{j,j'=1}^{N}, \qquad B_{\varepsilon,jj'}(k,\theta)\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \\ &C_{\varepsilon,j'}(k,\theta)\colon L^2(\hat{\Gamma}) \to L^2(\mathbb{R}^3); \qquad \varepsilon \geq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \\ &\qquad\qquad \theta \in \hat{\Lambda}, \quad j,j' = 1, \ldots, N, \end{aligned} \tag{1.4.129}$$

with integral kernels

$$\begin{aligned} A_{\varepsilon,j}(k,\theta,v,x) &= g_k(v - \varepsilon x - y_j, \theta) v_j(x), \\ B_{\varepsilon,jj'}(k,\theta,x,x') &= \varepsilon\lambda_j(\varepsilon) u_j(x) g_k(\varepsilon(x - x') + y_j - y_{j'}, \theta) v_{j'}(x'), \\ C_{\varepsilon,j'}(k,\theta,x,v) &= \lambda_{j'}(\varepsilon) u_{j'}(x) g_k(\varepsilon x + y_{j'} - v, \theta), \\ &\varepsilon \geq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad x, x' \in \mathbb{R}^3, \\ &v \in \hat{\Gamma}, \quad \theta \in \hat{\Lambda}, \quad j,j' = 1, \ldots, N. \end{aligned} \tag{1.4.130}$$

PROOF. It suffices to prove

$$\tilde{\mathcal{U}}(H_{\varepsilon,Y+\Lambda} - k^2)^{-1} \tilde{\mathcal{U}}^{-1} = |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta (H_{\varepsilon,\Lambda,Y}(\theta) - k^2)^{-1},$$

$$k^2 \in \mathbb{C} - \mathbb{R}, \tag{1.4.131}$$

where $H_{\varepsilon,\Lambda,Y}(\theta)$ is introduced above. Having defined all necessary operators, one easily verifies that

$$\tilde{\mathcal{U}} G_k = \left[|\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, g_k(\theta) \right] \tilde{\mathcal{U}}, \qquad \operatorname{Im} k > 0, \tag{1.4.132}$$

and furthermore that

$$\tilde{\mathscr{U}} A_{\varepsilon,j}(k) = \left[|\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, A_{\varepsilon,j}(k,\theta) \right] \mathscr{F},$$

$$\tilde{\mathscr{F}}_\Lambda B_{\varepsilon,jj'}(k) = \left[|\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, B_{\varepsilon,jj'}(k,\theta) \right] \tilde{\mathscr{F}}_\Lambda,$$

$$\tilde{\mathscr{F}}_\Lambda C_{\varepsilon,j}(k) = \left[|\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, C_{\varepsilon,j}(k,\theta) \right] \tilde{\mathscr{U}};$$

$$\varepsilon > 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k > 0, \quad \theta \in \hat{\Lambda}, \quad j, j' = 1, \ldots, N, \qquad (1.4.133)$$

where $\tilde{F}_\Lambda$ is defined by (1.4.63) with $N = 1$, and $A_{\varepsilon,j}(k)$, $B_{\varepsilon,jj'}(k)$, and $C_{\varepsilon,j'}(k)$ are given by (1.2.4). Using (1.2.8) this proves the decomposition. ■

As one would expect the operator $(H_{\varepsilon,\Lambda,Y}(\theta) - k^2)^{-1}$ converges to $(-\Delta_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1}$, the decomposition of $(-\Delta_{\alpha,Y+\Lambda} - k^2)^{-1}$, as $\varepsilon \downarrow 0$:

Theorem 1.4.8. *Let $V_j \in R$,* supp V_j *compact, be real-valued and let $\lambda_j(\varepsilon) = 1 + \varepsilon\lambda_j'(0) + o(\varepsilon)$ as $\varepsilon \downarrow 0, j = 1, \ldots, N$. Assume that $\lambda_j'(0) \neq 0$ if $H_j = -\Delta \dotplus V_j$ is in case* III *or* IV. *Then $H_{\varepsilon,\Lambda,Y}(\theta)$ converges in norm resolvent sense to $-\Delta_{\alpha,\Lambda,Y}(\theta)$, viz.*

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\varepsilon,\Lambda,Y}(\theta) - k^2)^{-1} = (-\Delta_{\alpha,\Lambda,Y}(\theta) - k^2)^{-1},$$

$$k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \quad \theta \in \hat{\Lambda}, \qquad (1.4.134)$$

where

$$\alpha_j = \begin{cases} \infty & \textit{in case } \mathrm{I}, \\ -\lambda_j'(0) |(v_j, \phi_j)|^{-2} & \textit{in case } \mathrm{II}, \\ \infty & \textit{in case } \mathrm{III}, \\ -\lambda_j'(0) \left\{ \sum_{l=1}^{N_j} |(v_j, \phi_{jl})|^2 \right\}^{-1} & \textit{in case } \mathrm{IV}. \end{cases} \qquad (1.4.135)$$

Remark. If $\alpha_{j_0} = \infty$ for some $j_0 \in \{1, \ldots, N\}$, then the j_0th row and line should be removed in $\Gamma_{\alpha,\Lambda,Y}(k,\theta)$, i.e., there is no point interaction at y_{j_0}.

PROOF. Again our basic tool in proving (1.4.134) is to study the explicit expressions (1.4.128) and (1.4.57) for the resolvents of $H_{\varepsilon,\Lambda,Y}(\theta)$ and $-\Delta_{\alpha,\Lambda,Y}(\theta)$, respectively. We have the asymptotic expansions

$$B_{\varepsilon,jj'}(k,\theta) = D_{jj'} + \varepsilon E_{jj'}(k,\theta) + o(\varepsilon) \qquad (1.4.136)$$

valid in Hilbert–Schmidt norm as $\varepsilon \downarrow 0$ where

$$\begin{aligned} D_{jj'} &= \delta_{jj'} u_j G_0 v_j, \\ E_{jj'}(k,\theta) &= g_k(y_j - y_{j'}, \theta)(v_{j'}, \cdot) u_j; \qquad j, j' = 1, \ldots, N. \end{aligned} \qquad (1.4.137)$$

The rest of the proof is identical to that of Theorem II.1.2.4. ■

This result will be applied to the analysis of the behavior of the spectrum of $H_{\varepsilon,\Lambda,Y}(\theta)$ in the limit $\varepsilon \downarrow 0$. The first result treats the case $Y = \{0\}$.

Theorem 1.4.9. *Let $V \in R$, supp V compact, be real-valued and let $\lambda(\varepsilon)$, $\lambda(0) = 1$, be analytic in a neighborhood of zero. Assume $H = -\Delta \dotplus V$ to be in case* II *or* IV *and suppose* (I.1.2.84) *and $\lambda'(0) \neq 0$ in case* IV. *Assume that $E_\varepsilon(\theta)$, $\theta \in \hat{\Lambda}$, is an eigenvalue of $H_{\varepsilon,\Lambda}(\theta) \equiv H_{\varepsilon,\Lambda,\{0\}}(\theta)$, chosen to be continuous in ε, $\varepsilon > 0$, which remains bounded for $\varepsilon > 0$ small. Then*

$$E_0(\theta) = \lim_{\varepsilon \downarrow 0} E_\varepsilon(\theta), \qquad \theta \in \hat{\Lambda}, \tag{1.4.138}$$

exists and is an eigenvalue of $-\Delta_{\alpha,\Lambda}(\theta)$, $-\Delta_{\alpha,\Lambda}(\theta)$ being the norm resolvent limit of $H_{\varepsilon,\Lambda}(\theta)$ as $\varepsilon \downarrow 0$. Assume this eigenvalue to be in case (a) *of the proof of Theorem* 1.4.4. *Then*

$$E_\varepsilon(\theta) = E_0(\theta) + \varepsilon E_1(\theta) + o(\varepsilon), \tag{1.4.139}$$

where

$$E_1(\theta) = h_\Lambda(E_0(\theta), \theta)[A + E_0(\theta)B], \qquad \theta \in \hat{\Lambda}. \tag{1.4.140}$$

In case II

$$\begin{aligned} A &= \tfrac{1}{2}\lambda''(0) + \lambda'(0)^2 + \lambda'(0)(\tilde{\phi}, \chi), \\ B &= (8\pi)^{-1} \iint_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)} v(x) |x - x'| \phi(x') v(x'), \\ h_\Lambda(E_0(\theta), \theta) &= |\hat{\Gamma}| \left\{ \sum_{\gamma \in \Gamma} \frac{1}{[|\gamma + \theta|^2 - E_0(\theta)]^2} \right\}^{-1}, \end{aligned} \tag{1.4.141}$$

where χ is given by (1.4.146). *In case* IV, *ϕ (resp. $\tilde{\phi}$) should be replaced by ϕ_1 (resp. $\tilde{\phi}_1$). $E_\varepsilon(\theta)$ is analytic in ε near $\varepsilon = 0$ if $E_0(\theta) < 0$.*

PROOF. If $E_0(\theta) = \lim_{\varepsilon \downarrow 0} E_\varepsilon(\theta)$ (which exists due to the norm resolvent convergence and the discrete spectrum of the limit operator) is negative, we can follow the proof of Theorem II.1.3.1 to obtain the stated expansion. In fact, using (1.4.38) we see that $B_\varepsilon(k, \theta)$ is analytic in ε and k and we can follow the analysis in the proof of Theorem II.1.3.1 with $G_k(x)$ replaced by $g_k(x, \theta)$. Recall that by Theorem 1.4.4 $E_0(\theta)$ is a simple eigenvalue and $N = 1$ in the notation of Theorem II.1.3.1. (Hence the analysis from Part I would also apply here.) If, however, $E_0(\theta) \geq 0$ (which by assumption is still simple), we are not able to conclude that $B_\varepsilon(k, \theta)$ is analytic in ε in a neighborhood of zero. But $B_\varepsilon(k, \theta)$ remains a Hilbert–Schmidt operator when $k^2 \geq 0$, $k^2 \notin |\Gamma + \theta|^2$ because

$$\begin{aligned} B_\varepsilon(k, \theta, x, x') &= \varepsilon(k^2 - \tilde{k}^2)|\hat{\Gamma}|^{-1} u(x) \sum_{\gamma \in \Gamma} \frac{e^{i(\gamma+\theta)[\varepsilon(x-x')]}}{(|\gamma + \theta|^2 - k^2)(|\gamma + \theta|^2 - \tilde{k}^2)} v(x') \\ &\quad + \varepsilon u(x) \sum_{\lambda \in \Lambda} \tilde{G}_{\tilde{k}}(\varepsilon(x - x') + \lambda) e^{-i\theta\lambda} v(x') \end{aligned} \tag{1.4.142}$$

for any $\tilde{k} \in \mathbb{C}$, Im $\tilde{k} > 0$, cf. Lemma 1.4.2, and in a similar way $B_\varepsilon(k, \theta)$ is easily seen to be two times continuously differentiable in Hilbert–Schmidt norm in ε and k.

Hence $E_\varepsilon(\theta)$ has the form

$$E_\varepsilon(\theta) = E_0(\theta) + \varepsilon E_1(\theta) + o(\varepsilon). \tag{1.4.143}$$

The projection $P_\varepsilon(\theta)$ onto the eigenspace of the operator $B_\varepsilon((E_\varepsilon(\theta))^{1/2}, \theta)$ to the eigenvalue -1 can be chosen to be two times differentiable in norm with respect to ε [251]. Defining

$$\phi_\varepsilon(\theta) = P_\varepsilon(\theta)\phi, \tag{1.4.144}$$

where ϕ is an eigenvector of $B_0((E_0(\theta))^{1/2}, \theta) = uG_0v$ with eigenvalue -1, we expand the equation

$$[1 + B_\varepsilon((E_\varepsilon(\theta))^{1/2}, \theta)]\phi_\varepsilon(\theta) = 0 \tag{1.4.145}$$

with respect to ε to obtain the stated form of $E_1(\theta)$ with

$$\chi = T[\lambda'(0)\phi - \alpha(v, \phi)u], \tag{1.4.146}$$

T being the reduced resolvent of $1 + uG_0v$, cf. (I.1.2.37). ■

Recall from Theorems 1.4.4 and 1.4.5 that each eigenvalue in case (a) gives rise to a band when θ varies in $\hat{\Lambda}$. The bands are connected at points $E(\tilde{\theta})$ where there exist at least three points $\gamma_1, \gamma_2, \gamma_3 \in \Gamma$ with $E(\tilde{\theta}) = |\gamma_1 + \tilde{\theta}|^2 = |\gamma_2 + \tilde{\theta}|^2 = |\gamma_3 + \tilde{\theta}|^2$. From (1.4.140) we see that $E_1(\theta) \to 0$ when $\theta \to \tilde{\theta}$. Thus we see that in this sense the bands do not open up to first order in ε.

Our last result in this section concerns the behavior of the negative part of the spectrum in the case where Y consists of N points.

Theorem 1.4.10. *Let $V_j \in R$, supp V_j compact, be real-valued and let $\lambda_j(\varepsilon)$ be real analytic in a neighborhood of zero, $\lambda_j(0) = 1, j = 1, \ldots, N$. Fix $\theta \in \hat{\Lambda}$ and assume $E_\varepsilon(\theta)$ to be an eigenvalue of $H_{\varepsilon,\Lambda,Y}(\theta)$ such that*

$$-\infty < M_1 \le E_\varepsilon(\theta) \le M_2 < 0 \tag{1.4.147}$$

for $\varepsilon > 0$ small enough. Let $\{\varepsilon_n\}$ be a positive sequence decreasing to zero, and let $E_0(\theta)$ be an accumulation point of $\{E_{\varepsilon_n}(\theta)\}$. Then $E_0(\theta)$ is an eigenvalue of $-\Delta_{\alpha,\Lambda,Y}(\theta)$, $-\Delta_{\alpha,\Lambda,Y}(\theta)$ being the limit of $H_{\varepsilon,\Lambda,Y}(\theta)$ in norm resolvent sense as $\varepsilon \downarrow 0$. Let $M(\theta)$ be the multiplicity of the eigenvalue $E_0(\theta)$. Then there exist functions $h_l(\theta)$, analytic near the origin, $h_l(\theta, 0) = 0$, and integers $m_l(\theta) \in \{1, 2\}$, $l = 1, \ldots, m(\theta)$, such that

$$\begin{aligned} E_\varepsilon(\theta) &= E_0(\theta) + h_l(\theta, \varepsilon^{1/m_l(\theta)}) \\ &= E_0(\theta) + \sum_{r=1}^{\infty} a_{l,r}(\theta)\varepsilon^{r/m_l(\theta)}, \qquad l = 1, \ldots, m(\theta), \quad \sum_{l=1}^{m(\theta)} m_l(\theta) = M(\theta), \end{aligned} \tag{1.4.148}$$

are all the eigenvalues of $H_{\varepsilon,\Lambda,Y}(\theta)$ near $E_0(\theta)$ for $\varepsilon > 0$ sufficiently small. If $m_l(\theta) = 2$ for some l, both square roots should be used such that the total multiplicity of all eigenvalues equals $M(\theta)$.

Proof. The proof is similar to that of Theorem II.1.3.1 except that $G_k(x)$ has to be replaced by $g_k(x, \theta)$. ■

III.1.5 Straight Polymers

Replacing the three-dimensional lattice Λ from the preceding section by a one-dimensional lattice Λ_1, viz.

$$\Lambda_1 = \{(0, 0, na) \in \mathbb{R}^3 | n \in \mathbb{Z}\}, \qquad a > 0, \tag{1.5.1}$$

we obtain a one-electron model of an infinitely long straight polymer as explained in Sect. 1.3.

Our basic tools in studying this operator will again be Fourier analysis and the direct integral decomposition. In contrast to the discussion of the crystal we will use Theorem 1.1.1 to define the operator, and then make the integral decomposition directly.

The point interactions will be located at

$$Y_1 = Y + \Lambda_1, \tag{1.5.2}$$

where

$$Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}^3 \tag{1.5.3}$$

is such that the third component of each $y_j \in Y$ belongs to $\hat{\Gamma}_1$, i.e.,

$$y_j = (y_j^1, y_j^2, y_j^3) \in Y, \qquad y_j^3 \in \hat{\Gamma}_1, \quad j = 1, \ldots, N, \tag{1.5.4}$$

where

$$\hat{\Gamma}_1 = \left[-\frac{a}{2}, \frac{a}{2}\right). \tag{1.5.5}$$

The dual lattice, Γ_1, and the dual group, $\hat{\Lambda}_1$, read, respectively,

$$\Gamma_1 = \left\{\left(0, 0, \frac{2\pi}{a} n\right) \in \mathbb{R}^3 \,\middle|\, n \in \mathbb{Z}\right\}, \qquad \hat{\Lambda}_1 = [-\pi/a, \pi/a). \tag{1.5.6}$$

Whenever convenient we shall identify Λ_1 and $\{na \in \mathbb{R} | n \in \mathbb{Z}\}$ and similarly for Γ_1. Furthermore, we will often write

$$(p, \gamma) = (p^1, p^2, \gamma) \in \mathbb{R}^3, \qquad p = (p^1, p^2) \in \mathbb{R}^2, \quad \gamma \in \Gamma_1. \tag{1.5.7}$$

The proper decomposition of $L^2(\mathbb{R}^3)$ for the polymer (cf. the operator $\mathscr{U}$ given by (1.4.16) in the crystal case), is now given by

$$\begin{aligned} &\mathscr{U}_1: L^2(\mathbb{R}^3) \to L^2(\hat{\Lambda}_1, L^2(\mathbb{R}^2 \times \Gamma_1)) = \int_{\hat{\Lambda}_1}^{\oplus} d\theta\, L^2(\mathbb{R}^2 \times \Gamma_1), \\ &(\mathscr{U}_1 f)(\theta, p, \gamma) = \hat{f}(p, \gamma + \theta), \quad \theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}^2, \quad \gamma \in \Gamma_1, \quad \hat{f} \in L^2(\mathbb{R}^3). \end{aligned} \tag{1.5.8}$$

Decomposing the free Hamiltonian $-\hat{\Delta}$ in p-space with respect to this decomposition we obtain for its resolvent the operator

$$\begin{aligned} &G_k(\theta): L^2(\mathbb{R}^2 \times \Gamma_1) \to L^2(\mathbb{R}^2 \times \Gamma_1), \\ &\quad (G_k(\theta)g)(p, \gamma) = [|(p, \gamma + \theta)|^2 - k^2]^{-1} g(p, \gamma), \\ &\quad\quad \theta \in \hat{\Lambda}_1, \quad k^2 \notin [\theta^2, \infty), \quad \operatorname{Im} k \geq 0. \end{aligned} \tag{1.5.9}$$

We will also need the function

$$g_k(x,\theta)=\begin{cases}\dfrac{ik}{4\pi}-e^{i\theta x}\left\{\dfrac{ik}{4\pi}+\dfrac{1}{4\pi a}\ln[2(\cos(ka)-\cos(\theta a))]\right\}, & x\in\Lambda_1,\\[2mm] \dfrac{e^{i\theta x^3}}{4\pi a}\left[2\beta\left(\dfrac{x^3}{a}\right)\cos\left(\dfrac{\pi x^3}{a}\right)+\dfrac{1}{2}\displaystyle\int_{(k-\theta)a}^{\pi}dt\,\dfrac{e^{i(x^3-1)t/2}}{\sin(t/2)}\right. & \\ \qquad\left.+\dfrac{1}{2}\displaystyle\int_{(k+\theta)a}^{\pi}dt\,\dfrac{e^{-i(x^3+1)t/2}}{\sin(t/2)}\right], & x=(0,0,x^3)\notin\Lambda_1,\\[2mm] 2\pi a\displaystyle\sum_{\gamma\in\Gamma_1}K_0\left(\sqrt{(\gamma+\theta)^2-k^2}\,|\tilde{x}|\right)e^{i(\gamma+\theta)x^3}, & \\ \qquad x=(\tilde{x},x^3)\in\mathbb{R}^3,\quad \tilde{x}\neq 0;\quad \theta\in\hat{\Lambda}_1, & \end{cases} \tag{1.5.10}$$

($\beta(\cdot)$ and $K_0(\cdot)$ being the beta function and modified Bessel function, respectively, [1]). The domain of definition of $g_k(x,\theta)$ as a function of the complex variable k is illustrated in Figure 6.

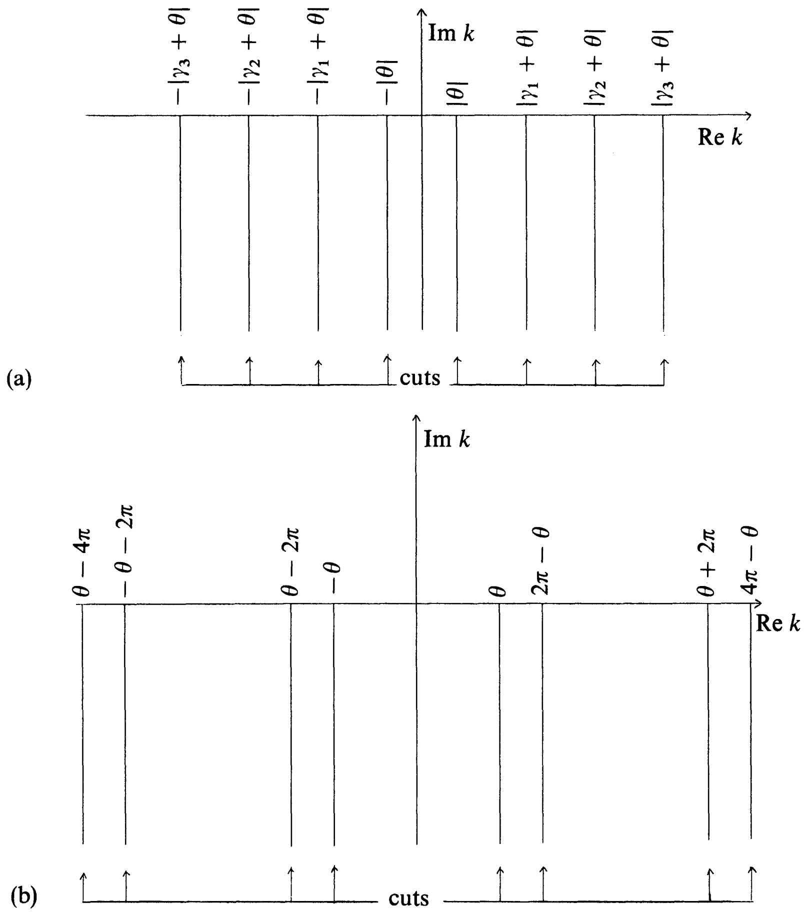


Figure 6 The domain of definition of the function $g_k(x,\theta)$, $\theta\in\hat{\Lambda}_1$, as a function of k in the complex k-plane: (a) when $x\in\Lambda_1$; (b) when $x\in\mathbb{R}^3-\Lambda_1$.

Furthermore, we will use, for the decomposition in x-space, the analog of $\tilde{\mathscr{U}}$ (cf. (1.4.53))

$$\tilde{\mathscr{U}}_1\colon \mathscr{S}(\mathbb{R}^3) \to L^2\left(\hat{\Lambda}_1, \frac{a}{2\pi}\, d\theta; L^2(\mathbb{R}^2 \times \hat{\Gamma}_1)\right) = \frac{a}{2\pi}\int_{\hat{\Lambda}_1}^{\oplus} d\theta\, L^2(\mathbb{R}^2 \times \hat{\Gamma}_1),$$

$$(\tilde{\mathscr{U}}_1 f)(\theta, p, \nu) = (2\pi)^{-1} \sum_{\lambda \in \Lambda_1} \int_{\mathbb{R}^2} d^2x\, f(x, \lambda + \nu) e^{-ipx} e^{-i\theta\lambda},$$

$$\theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}^2, \quad \nu \in \hat{\Gamma}_1, \quad f \in \mathscr{S}(\mathbb{R}^3), \tag{1.5.11}$$

and then extend $\tilde{\mathscr{U}}_1$ to $L^2(\mathbb{R}^3)$ by continuity. The extension is still denoted by $\tilde{\mathscr{U}}_1$.

Theorem 1.5.1. *Let $y_j \in Y$, $y_j^3 \in \hat{\Gamma}_1$, and $\alpha_j \in \mathbb{R}$, $j = 1, \ldots, N$. Then the self-adjoint operator $-\hat{\Delta}_{\alpha, Y+\Lambda_1}$ in $L^2(\mathbb{R}^3)$ defined in Theorem 1.1.1, with $Y = \{y_1, \ldots, y_N\}$ and*

$$\alpha_{y_j+\lambda} = \alpha_j, \qquad j = 1, \ldots, N, \quad \alpha = \{\alpha_j\}, \quad \lambda \in \Lambda_1, \tag{1.5.12}$$

satisfies

$$\mathscr{U}_1[-\hat{\Delta}_{\alpha, Y+\Lambda_1}]\mathscr{U}_1^{-1} = \int_{\hat{\Lambda}_1}^{\oplus} d\theta[-\hat{\Delta}_{\alpha, \Lambda_1, Y}(\theta)], \tag{1.5.13}$$

where $-\hat{\Delta}_{\alpha, \Lambda_1, Y}(\theta)$ is the self-adjoint operator in $L^2(\mathbb{R} \times \Gamma_1)$ with resolvent

$$(-\hat{\Delta}_{\alpha, \Lambda_1, Y}(\theta) - k^2)^{-1} = G_k(\theta) + \sum_{j,j'=1}^{N} [\Gamma_{\alpha, \Lambda_1, Y}(k, \theta)]_{jj'}^{-1} (F_{-\bar{k}, y_{j'}}(\theta), \cdot) F_{k, y_j}(\theta),$$

$$k^2 \in \rho(-\hat{\Delta}_{\alpha, \Lambda_1, Y}(\theta)), \quad \operatorname{Im} k \geq 0, \ \theta \in \hat{\Lambda}_1, \ y_j^3 \in \hat{\Gamma}_1, \ \alpha_j \in \mathbb{R}, \ j = 1, \ldots, N, \tag{1.5.14}$$

where

$$\Gamma_{\alpha, \Lambda_1, Y}(k, \theta) = [\alpha_j \delta_{jj'} - g_k(y_j - y_{j'}, \theta)]_{j,j'=1}^{N}, \qquad \theta \in \hat{\Lambda}_1, \tag{1.5.15}$$

and

$$F_{k, y_j}(\theta, p, \gamma) = (2\pi)^{-3/2} \frac{e^{-i(p, \gamma+\theta) y_j}}{|(p, \gamma + \theta)|^2 - k^2},$$

$$k^2 \notin [\theta^2, \infty), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}^2, \quad \gamma \in \Gamma_1, \quad j = 1, \ldots, N. \tag{1.5.16}$$

If we introduce

$$-\Delta_{\alpha, Y+\Lambda_1} = \mathscr{F}^{-1}[-\hat{\Delta}_{\alpha, Y+\Lambda_1}]\mathscr{F}, \tag{1.5.17}$$

then

$$\tilde{\mathscr{U}}_1[-\Delta_{\alpha, Y+\Lambda_1}]\tilde{\mathscr{U}}_1^{-1} = \frac{a}{2\pi}\int_{\hat{\Lambda}_1}^{\oplus} d\theta[-\Delta_{\alpha, \Lambda_1, Y}(\theta)], \tag{1.5.18}$$

where $-\Delta_{\alpha, \Lambda_1, Y}(\theta)$ is the self-adjoint operator in $L^2(\mathbb{R}^2 \times \hat{\Gamma}_1)$ with resolvent

$$(-\Delta_{\alpha, \Lambda_1, Y}(\theta) - k^2)^{-1}$$

$$= g_k(\theta) + \sum_{j,j'=1}^{N} [\Gamma_{\alpha, \Lambda_1, Y}(k, \theta)]_{jj'}^{-1} (\overline{g_k(\cdot - y_{j'}, \theta)}, \cdot) g_k(\cdot - y_j, \theta),$$

$$k^2 \in \rho(-\Delta_{\alpha, \Lambda_1, Y}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_1, \tag{1.5.19}$$

where

$$g_k(\theta)\colon L^2(\mathbb{R}^2 \times \hat{\Gamma}_1) \to L^2(\mathbb{R}^2 \times \hat{\Gamma}_1),$$

$$(g_k(\theta)f)(p, v) = \int_{\mathbb{R}^2} d^2p' \int_{\hat{\Gamma}_1} d^2v'\, g_k((p - p', v - v'), \theta) f(p', v'),$$

$$k^2 \notin [\theta^2, \infty), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}^2, \quad v \in \hat{\Gamma}_1, \quad f \in L^2(\mathbb{R}^2 \times \hat{\Gamma}_1), \tag{1.5.20}$$

and $g_k(x, \theta)$ *is given by* (1.5.10).

PROOF. Following the proof of Theorem 1.4.3 we get (1.5.13) where $(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta) - k^2)^{-1}$ equals (1.5.14) with

$$\Gamma_{\alpha,\Lambda_1,Y}(k, \theta) = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \sum_{\lambda \in \Lambda_1} \tilde{G}_k(y_j - y_{j'} + \lambda) e^{-i\theta\lambda}\right]_{j,j'=1}^{N}. \tag{1.5.21}$$

Next we observe that the infinite sum on the diagonal actually can be summed to yield (1.5.15) while the off-diagonal sum can be summed ([237], eq. (14.3.1) and (17.3.1)) when $y_j - y_{j'} = (0, 0, y_j^3 - y_{j'}^3) \notin \Lambda_1$ and can be expressed in terms of $K_0(\cdot)$ when $y_j - y_{j'} = (\tilde{y}_j - \tilde{y}_{j'}, y_j^3 - y_{j'}^3)$, $\tilde{y}_j - \tilde{y}_{j'} \neq 0$ ([333], p. 62). The rest of the proof is similar to that of Theorem 1.4.3. ■

Since we will use later on detailed properties of the domain $\mathscr{D}(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta))$ of $-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta)$ we give the following

Theorem 1.5.2. *Let* $y_j \in Y$, $y_j^3 \in \hat{\Gamma}_1$, $\alpha_j \in \mathbb{R}$, $j = 1, \ldots, N$, *and* $\theta \in \hat{\Lambda}_1$. *Then the domain* $\mathscr{D}(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta))$ *of* $-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta)$ *consists of all functions* $\psi(\theta)$ *such that*

$$\psi(\theta, p, \gamma) = \phi_k(\theta, p, \gamma) + \sum_{j=1}^{N} a_j(k, \theta) F_{k,y_j}(\theta, p, \gamma),$$

$$p \in \mathbb{R}^2, \quad \gamma \in \Gamma_1, \tag{1.5.22}$$

where

$$a_j(k, \theta) = \sum_{j'=1}^{N} [\Gamma_{\alpha,\Lambda_1,Y}(k, \theta)]_{jj'}^{-1} \sum_{\gamma \in \Gamma_1} \int_{\mathbb{R}^2} d^2p\, e^{i(p,\gamma+\theta)y_{j'}} \phi_k(\theta, p, \gamma). \tag{1.5.23}$$

Here $k^2 \in \rho(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta))$, $\operatorname{Im} k \geq 0$, *and*

$$\phi_k(\theta) \in \mathscr{D}(|(p, \gamma + \theta)|^2)$$

$$= \left\{ g \in L^2(\mathbb{R}^2 \times \Gamma_1) \,\middle|\, \sum_{\gamma \in \Gamma_1} \int_{\mathbb{R}^2} d^2p\, |(p, \gamma + \theta)|^4 |g(p, \gamma)|^2 < \infty \right\}. \tag{1.5.24}$$

This decomposition is unique, and with $\psi(\theta)$ *of this form we have*

$$[(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta) - k^2)\psi(\theta)](p, \gamma) = [|(p, \gamma + \theta)|^2 - k^2]\phi_k(p, \gamma). \tag{1.5.25}$$

PROOF. Similar to that of Theorem II.1.1.3. ■

We now turn to the analysis of spectral properties, starting with the operator $-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta)$. For this operator we encounter resonances and, in particular, real resonances. Here resonances are defined in the following way: $k_0 \in \mathbb{C}$, $\operatorname{Im} k_0 \leq 0$, is a resonance of $-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta)$ iff $\det[\Gamma_{\alpha,\Lambda_1,Y}(k_0, \theta)] = 0$ and, if $k_0 \in (0, \infty)$, then $k_0^2 \notin \sigma_p(-\hat{\Delta}_{\alpha,\Lambda_1,Y}(\theta))$. The multiplicity of k_0 by definition equals the multiplicity of the zero of $\det[\Gamma_{\alpha,\Lambda_1,Y}(k, \theta)]$ at $k = k_0$.

From now on we will assume that Y consists of only one point which by translation can be taken to be zero.

Theorem 1.5.3. *Let $\alpha \in \mathbb{R}$, and $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta) \equiv -\hat{\Delta}_{\alpha,\Lambda_1,\{0\}}(\theta)$, $\theta \in \hat{\Lambda}_1$. Then the essential spectrum of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ is purely absolutely continuous and equals*

$$\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \sigma_{\text{ac}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = [\theta^2, \infty), \qquad \sigma_{\text{sc}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \varnothing, \qquad \theta \in \hat{\Lambda}_1. \tag{1.5.26}$$

Writing

$$z^{\alpha,\Lambda_1}(\theta) = \cos(\theta a) + \tfrac{1}{2} e^{-4\pi a \alpha}, \tag{1.5.27}$$

we have

$$\sigma_p(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \begin{cases} \{-a^{-2} \ln^2[z^{\alpha,\Lambda_1}(\theta) + \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}]\}, & z^{\alpha,\Lambda_1}(\theta) > 1, \\ \{a^{-2} \arccos^2[z^{\alpha,\Lambda_1}(\theta)]\}, & z^{\alpha,\Lambda_1}(\theta) \leq 1 \text{ and } \arccos^2[z^{\alpha,\Lambda_1}(\theta)] < (a\theta)^2, \\ \varnothing, & z^{\alpha,\Lambda_1}(\theta) \leq 1 \text{ and } \arccos^2[z^{\alpha,\Lambda_1}(\theta)] \geq (a\theta)^2. \end{cases} \tag{1.5.28}$$

If $E^{\alpha,\Lambda_1}(\theta)$ is an eigenvalue of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$, i.e., $E^{\alpha,\Lambda_1}(\theta) \in \sigma_p(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta))$, then $E^{\alpha,\Lambda_1}(\theta)$ is simple ($E^{\alpha,\Lambda_1}(\theta) < \theta^2$) and the corresponding eigenfunction equals

$$\psi_{E^{\alpha,\Lambda_1}(\theta)}(\theta, p, \gamma) = [|(p, \gamma + \theta)|^2 - E^{\alpha,\Lambda_1}(\theta)]^{-1}, \qquad \theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}^2, \quad \gamma \in \Gamma_1. \tag{1.5.29}$$

$E^{\alpha,\Lambda_1}(\theta)$ is strictly increasing in α for $\theta \in \hat{\Lambda}_1$. In addition, $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ has the following resonances, all of which are simple.

If $z^{\alpha,\Lambda_1}(\theta) \leq 1$, then

$$k_n^{\alpha,\Lambda_1}(\theta) = \{\pm\arccos[z^{\alpha,\Lambda_1}(\theta)] + 2\pi n\}/a, \qquad n \in \mathbb{Z} - \{0\}, \tag{1.5.30}$$

are simple resonances of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$. If $k_0^{\alpha,\Lambda_1}(\theta)^2 \geq \theta^2$ allowing $n = 0$ in (1.5.30), then also $k_0^{\alpha,\Lambda_1}(\theta)$ is a simple resonance.

If $z^{\alpha,\Lambda_1}(\theta) > 1$, then

$$k_n^{\alpha,\Lambda_1}(\theta) = \{-i \ln[z^{\alpha,\Lambda_1}(\theta) + \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}] + 2\pi n\}/a, \qquad n \in \mathbb{Z}, \tag{1.5.31}$$

are simple resonances of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$. $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ has no other eigenvalues or resonances.

Remark. Observe that we have an infinite sequence of real resonances provided $z^{\alpha,\Lambda_1}(\theta) \le 1$, while all the resonances are complex when $z^{\alpha,\Lambda_1}(\theta) > 1$.

PROOF. $\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = [\theta^2, \infty)$ follows from Weyl's theorem ([391], Theorem XIII.14). Using Theorem XIII.20, [391], we see that $\sigma_{\text{sc}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \varnothing$. The resonances and/or eigenvalues are solutions of

$$\alpha = g_k(0, \theta), \tag{1.5.32}$$

or equivalently, of

$$\cos(ka) = z^{\alpha,\Lambda_1}(\theta), \tag{1.5.33}$$

where $z^{\alpha,\Lambda_1}(\theta)$ is defined by (1.5.27). If $z^{\alpha,\Lambda_1}(\theta) \le 1$, the solutions of (1.5.27) are

$$k_n^{\alpha,\Lambda_1}(\theta) = \{\pm\arccos[z^{\alpha,\Lambda_1}(\theta)] + 2\pi n\}/a, \qquad n \in \mathbb{Z}, \tag{1.5.34}$$

and by considering the residuum of the resolvent at $[k_0^{\alpha,\Lambda_1}(\theta)]^2$ we find that $[k_0^{\alpha,\Lambda_1}(\theta)]^2$ is a simple eigenvalue with the stated eigenfunction (1.5.29) provided $[k_0^{\alpha,\Lambda_1}(\theta)]^2 < \theta^2$, i.e., if $[k_0^{\alpha,\Lambda_1}(\theta)]^2$ stays away from the essential spectrum. All $[k_n^{\alpha,\Lambda_1}(\theta)]^2$ for $n \in \mathbb{Z} - \{0\}$ (and also $[k_0^{\alpha,\Lambda_1}(\theta)]^2$ if $[k_0^{\alpha,\Lambda_1}(\theta)]^2 \ge \theta^2$) are embedded in the essential spectrum, and we will show that $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ has no embedded eigenvalues. Assume that $\psi(\theta)$ is an eigenvector to the eigenvalue $E(\theta)$, $E(\theta) = [k(\theta)]^2 \ge \theta^2$, i.e.,

$$-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)\psi(\theta) = E(\theta)\psi(\theta). \tag{1.5.35}$$

Applying Theorem 1.5.2, $\psi(\theta)$ can be written as

$$\psi(\theta, p, \gamma) = \phi_k(\theta, p, \gamma) + (2\pi)^{-2}a^{-1}[\alpha - g_k(0, \theta)]^{-1} \sum_{\gamma' \in \Gamma_1} \int_{\mathbb{R}^2} d^2p'\, \phi_k(\theta, p', \gamma') \cdot$$
$$\cdot [|(p, \gamma, \theta)|^2 - k^2]^{-1}, \qquad p \in \mathbb{R}^2, \quad \gamma \in \Gamma_1, \tag{1.5.36}$$

for some $k^2 \in \rho(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta))$, $\operatorname{Im} k > 0$, where

$$\begin{aligned}[E(\theta) - k^2]\psi(\theta, p, \gamma) &= [(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta) - k^2)\psi(\theta)](p, \gamma) \\ &= [|(p, \gamma + \theta)|^2 - k^2]\phi_k(\theta, p, \gamma).\end{aligned} \tag{1.5.37}$$

Hence

$$\phi_k(\theta, p, \gamma) = [E(\theta) - k^2][|(p, \gamma + \theta)|^2 - k^2]^{-1}\psi(\theta, p, \gamma). \tag{1.5.38}$$

Inserting (1.5.36) into (1.5.38) we find

$$\phi_k(\theta, p, \gamma) = (2\pi)^{-2}a^{-1}[\alpha - g_k(0, \theta)]^{-1} \sum_{\gamma' \in \Gamma_1} \int_{\mathbb{R}^2} d^2p'\, \phi_k(\theta, p', \gamma') \cdot$$
$$\cdot \{[|(p, \gamma + \theta)|^2 - E(\theta)]^{-1} - [|(p, \gamma + \theta)|^2 - k^2]^{-1}\} \tag{1.5.39}$$

which cannot be in $\mathscr{D}(|(p, \gamma + \theta)|^2)$ unless $\phi_k(\theta) = 0$ implying $\psi(\theta) = 0$.

If $z^{\alpha,\Lambda_1}(\theta) > 1$, we have to look for complex solutions of (1.5.33). Writing

$$\eta = e^{iak}, \tag{1.5.40}$$

we see that η satisfies

$$\eta^2 - 2z^{\alpha,\Lambda_1}(\theta)\eta + 1 = 0, \tag{1.5.41}$$

implying that

$$\eta_{\pm} = z^{\alpha,\Lambda_1}(\theta) \pm \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}. \tag{1.5.42}$$

Hence

$$k_n^{\alpha,\Lambda_1}(\theta) = \{-i \ln[z^{\alpha,\Lambda_1}(\theta) + \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}] + 2\pi n\}/a, \qquad n \in \mathbb{Z}, \tag{1.5.43}$$

and, in addition,

$$k^{\alpha,\Lambda_1}(\theta) = (i/a) \ln\{z^{\alpha,\Lambda_1}(\theta) + \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}\} \tag{1.5.44}$$

provide all solutions of (1.5.33). All $k_n^{\alpha,\Lambda_1}(\theta)$, $n \in \mathbb{Z}$, are complex resonances, while $E^{\alpha,\Lambda_1}(\theta) = [k^{\alpha,\Lambda_1}(\theta)]^2$ is a simple negative eigenvalue with eigenfunction (1.5.29). ∎

We now apply this theorem to analyze the spectrum of

$$\mathscr{U}_1[-\hat{\Delta}_{\alpha,\Lambda_1}]\mathscr{U}_1^{-1} = \int_{\hat{\Lambda}_1}^{\oplus} d\theta[-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)].$$

Theorem 1.5.4. *Let $\alpha \in \mathbb{R}$, and consider*

$$\mathscr{U}_1[-\hat{\Delta}_{\alpha,\Lambda_1}]\mathscr{U}_1^{-1} = \int_{\hat{\Lambda}_1}^{\oplus} d\theta[-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)]. \tag{1.5.45}$$

Then the essential spectrum of $-\hat{\Delta}_{\alpha,\Lambda_1}$ is purely absolutely continuous and equals

$$\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda_1}) = \sigma_{\text{ac}}(-\hat{\Delta}_{\alpha,\Lambda_1}) = \begin{cases} [E_-^{\alpha,\Lambda_1}, \infty), & \alpha \geq -(\ln 2)/2\pi a, \\ [E_-^{\alpha,\Lambda_1}, E_+^{\alpha,\Lambda_1}] \cup [0, \infty), & \alpha < -(\ln 2)/2\pi a, \end{cases}$$

$$\sigma_{\text{sc}}(-\hat{\Delta}_{\alpha,\Lambda_1}) = \varnothing, \tag{1.5.46}$$

where

$$E_{\pm}^{\alpha,\Lambda_1} = -a^{-2}\{\ln[\mp 1 + \tfrac{1}{2}e^{-4\pi a\alpha} + e^{-2\pi a\alpha}\sqrt{\tfrac{1}{4}e^{-4\pi a\alpha} \mp 1}]\}^2. \tag{1.5.47}$$

The spectrum of $-\hat{\Delta}_{\alpha,\Lambda_1}$ is monotone increasing in α in the sense that $\partial E_{\pm}^{\alpha,\Lambda_1}/\partial\alpha > 0$.

PROOF. If $\alpha < -(\ln 2)/2\pi a$, then $z^{\alpha,\Lambda_1}(\theta) > 1$ for all $\theta \in \hat{\Lambda}_1$. Hence the unique negative band is obtained by varying θ in $\hat{\Lambda}_1$ in the lowest eigenvalue

$$E^{\alpha,\Lambda_1}(\theta) = -a^{-2}\{\ln[z^{\alpha,\Lambda_1}(\theta) + \sqrt{[z^{\alpha,\Lambda_1}(\theta)]^2 - 1}]\}^2 \tag{1.5.48}$$

of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$. Together with Theorem XIII.87 in [391] and [85], Ch. 10, this proves the statements when $\alpha < -(\ln 2)/2\pi a$. If $\alpha \geq -(\ln 2)/2\pi a$, we can still find a nonempty open subset A of $\hat{\Lambda}_1$ such that $z^{\alpha,\Lambda_1}(\theta) > 1$ for $\theta \in A$. As $z^{\alpha,\Lambda_1}(\theta) \downarrow 1$, the eigenvalue (1.5.48) increases to zero, which proves that there is no gap in the spectrum when $\alpha \geq -(\ln 2)/2\pi a$. ∎

Our last topic in this section will be the ε-approximation in connection with $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$. For simplicity, we will only discuss the case $Y = \{0\}$, and start by introducing some notations. Let

$$\begin{aligned} &A_\varepsilon(k, \theta)\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^2 \times \hat{\Gamma}_1), \\ &B_\varepsilon(k, \theta)\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \\ &C_\varepsilon(k, \theta)\colon L^2(\mathbb{R}^2 \times \hat{\Gamma}_1) \to L^2(\mathbb{R}^3), \end{aligned} \tag{1.5.49}$$

be Hilbert–Schmidt operators with integral kernels

$$A_\varepsilon(k, \theta, \tilde{x}, v, x) = g_k((\tilde{x}, v) - \varepsilon x, \theta)v(x),$$
$$B_\varepsilon(k, \theta, x, x') = \varepsilon\lambda(\varepsilon)u(x)g_k(\varepsilon(x - x'), \theta)v(x'),$$
$$C_\varepsilon(k, \theta, x, \tilde{x}, v) = \lambda(\varepsilon)u(x)g_k(\varepsilon x - (\tilde{x}, v), \theta);$$
$$\varepsilon \geq 0, \quad k^2 \notin [\theta^2, \infty), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_1, \quad x, x' \in \mathbb{R}^3, \quad \tilde{x} \in \mathbb{R}^2, \quad v \in \hat{\Gamma}_1. \tag{1.5.50}$$

Theorem 1.5.5. *Let $V \in R$, supp V compact, $\lambda(\varepsilon) = 1 + \varepsilon\lambda'(0) + O(\varepsilon^2)$ as $\varepsilon \downarrow 0$ both be real-valued. Then the self-adjoint operator*

$$H_{\varepsilon,\Lambda_1} = -\Delta \dotplus \varepsilon^{-2}\lambda(\varepsilon) \sum_{\lambda \in \Lambda_1} V((\cdot - \lambda)/\varepsilon), \qquad \varepsilon > 0, \tag{1.5.51}$$

in $L^2(\mathbb{R}^3)$ can be decomposed as

$$\tilde{\mathscr{U}}_1 H_{\varepsilon,\Lambda_1} \tilde{\mathscr{U}}_1^{-1} = \frac{a}{2\pi} \int_{\hat{\Lambda}_1}^{\oplus} d\theta\, H_{\varepsilon,\Lambda_1}(\theta), \qquad \varepsilon > 0, \tag{1.5.52}$$

where $H_{\varepsilon,\Lambda_1}(\theta)$ is the self-adjoint operator on $L^2(\mathbb{R}^2 \times \hat{\Gamma}_1)$ with resolvent

$$(H_{\varepsilon,\Lambda_1}(\theta) - k^2)^{-1} = g_k(\theta) - \varepsilon A_\varepsilon(k, \theta)[1 + B_\varepsilon(k, \theta)]^{-1}C_\varepsilon(k, \theta),$$
$$\varepsilon > 0, \quad k^2 \in \rho(H_{\varepsilon,\Lambda_1}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_1. \tag{1.5.53}$$

Assume that $\lambda'(0) \neq 0$ if $H = -\Delta \dotplus V$ is in case III *or* IV. *Then $H_{\varepsilon,\Lambda_1}(\theta)$ converges in norm resolvent sense to the operator $-\Delta_{\alpha,\Lambda_1}(\theta)$ as $\varepsilon \downarrow 0$, i.e.,*

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\varepsilon,\Lambda_1}(\theta) - k^2)^{-1} = (-\hat{\Delta}_{\alpha,\Lambda_1}(\theta) - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \quad \theta \in \hat{\Lambda}_1, \tag{1.5.54}$$

where

$$\alpha = \begin{cases} \infty & \text{in case I}, \\ -\lambda'(0)|(v, \phi)|^{-2} & \text{in case II}, \\ \infty & \text{in case III}, \\ -\lambda'(0)\left[\sum_{j=1}^{N} |(v, \phi_j)|^2\right]^{-1} & \text{in case IV}. \end{cases} \tag{1.5.55}$$

Proof. The proof is similar to that of Theorems 1.4.8 and 1.4.9. ■

Remark. If $H = -\Delta \dotplus V$ is in case I or III, then

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\alpha,\Lambda_1}(\theta) - k^2)^{-1} = g_k(\theta), \qquad \theta \in \hat{\Lambda}_1, \quad k^2 \in \rho(-\hat{\Delta}(\theta)), \quad \operatorname{Im} k \geq 0, \tag{1.5.56}$$

where $g_k(\theta)$ is the resolvent of the free decomposed Laplacian $-\hat{\Delta}(\theta)$.

Applying the techniques from Sect. 1.4 and Sect. II.1.3, one can analyze the behavior of the at most one simple discrete eigenvalue and the complex resonances in the short-range approximation. However, the infinite straight polymer exhibits one very special feature, namely the existence of real resonances, i.e., poles of the resolvent $(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta) - k^2)^{-1}$ on the real k-axis in the limit $\varepsilon \downarrow 0$. In this context we define resonances of $H_{\varepsilon,\Lambda_1}(\theta)$ as follows: $k_0 \in \mathbb{C}$, $\operatorname{Im} k_0 \leq 0$, is a resonance of $H_{\varepsilon,\Lambda_1}(\theta)$ iff $\det_2[1 + B_\varepsilon(k_0, \theta)] = 0$ and, if $k_0 \in [0, \infty)$, then $k_0^2 \notin \sigma_p(H_{\varepsilon,\Lambda_1}(\theta))$. By definition the multiplicity of k_0 equals the multiplicity of the zero of $\det_2[1 + B_\varepsilon(k, \theta)]$ at $k = k_0$. We will show that, in general, the real resonances of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ also remain resonances for $H_{\alpha,\Lambda_1}(\theta)$ but to second order in ε they move into the "unphysical half-plane", i.e., they get a nonvanishing imaginary part. This is described in the following theorem, where for simplicity we assume $H = -\Delta \dotplus V$ to be in case II:

Theorem 1.5.6. *Let $V \in R$,* supp *V compact, be real-valued, and let $\lambda(\varepsilon)$ be real-analytic in ε for ε small, $\lambda(0) = 1$. Assume that $H = -\Delta \dotplus V$ is in case* II. *Let $E_0(\theta) = [k_0(\theta)]^2$, $\theta \in \hat{\Lambda}_1$, be any eigenvalue* ($\operatorname{Im} k_0(\theta) > 0$ *or* $k_0(\theta) < |\theta|$) *or resonance* ($\operatorname{Im} k_0(\theta) < 0$ *or* $k_0(\theta) \geq |\theta|$) *of $-\Delta_{\alpha,\Lambda_1}(\theta)$ as described in Theorem* 1.5.3 (*we omit the α and Λ_1 dependence in the notation*), *$-\Delta_{\alpha,\Lambda_1}(\theta)$ being the norm resolvent limit of $H_{\varepsilon,\Lambda_1}(\theta)$ as $\varepsilon \downarrow 0$. Then there exists a function $k_\varepsilon(\theta)$ for $\varepsilon > 0$ small enough with*

$$k_\varepsilon(\theta) = k_0(\theta) + \varepsilon k_1(\theta) + \varepsilon^2 k_2(\theta) + O(\varepsilon^3) \tag{1.5.57}$$

such that

$$\det_2[1 + B_\varepsilon(k_\varepsilon(\theta), \theta)] = 0, \qquad [\operatorname{Im} k_\varepsilon(\theta)]\cdot[\operatorname{Im} k_0(\theta)] \geq 0, \tag{1.5.58}$$

where

$$k_1(\theta) = 4\pi\frac{\cos[k_0(\theta)a] - \cos(\theta a)}{\sin[k_0(\theta)a]}\{A_1 + [k_0(\theta)]^2 B_1\}, \tag{1.5.59}$$

and

$$\begin{aligned}
k_2(\theta) = 4\pi\frac{\cos[k_0(\theta)a] - \cos(\theta a)}{\sin[k_0(\theta)a]}\cdot \\
\cdot\Bigg\{&-\frac{i[k_0(\theta)]^3}{24|(v, \phi)|^2}\int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)}v(x)|x - x'|^2 v(x')\phi(x') \\
&+ 2k_0(\theta)k_1(\theta)B_1 + [k_1(\theta)]^2 C_1(k_0(\theta)) + \lambda'(0)[k_0(\theta)]^2 B_1 \\
&+ \{A_1 + [k_0(\theta)]^2 B_1\}\left[\lambda'(0) + \frac{(v, \chi)}{(v, \phi)}\right] \\
&+ |(v, \phi)|^{-2}\int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)}v(x)E_1(k_0(\theta), x - x')v(x')\chi(x') \\
&+ |(v, \phi)|^{-2}\int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)}v(x)F_1(k_0(\theta), x - x')v(x')\phi(x') \\
&+ D_1\Bigg\}.
\end{aligned} \tag{1.5.60}$$

Here

$$A_1 = -\alpha\frac{(v,\chi)}{(v,\phi)} + \lambda'(0)\frac{(\tilde{\phi},\chi)}{|(v,\phi)|^2} + \lambda''(0)\frac{(\tilde{\phi},\phi)}{|(v,\phi)|^2} - \lambda'(0)\alpha,$$

$$B_1 = -\frac{1}{8\pi|(v,\phi)|^2}\int\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)}v(x)|x-x'|v(x')\phi(x'),$$

$$C_1(k) = \frac{a[1-\cos(ka)+\sin(ka)]\cos(\theta a)}{4\pi[\cos(ka)-\cos(\theta a)]^2},$$

$$D_1 = -\tfrac{1}{6}\lambda'''(0)\frac{(\tilde{\phi},\phi)}{|(v,\phi)|^2} + \tfrac{1}{2}\lambda'(0)\frac{(\tilde{\phi},\eta)}{|(v,\phi)|^2} - \lambda'(0)\alpha\frac{(v,\chi)}{(v,\phi)} - \lambda'''(0)\alpha + \tfrac{1}{2}\alpha\frac{(v,\eta)}{(v,\phi)},$$

$$E_1(k,x) = \left\{\frac{k}{ia}\ln\left[\frac{\sin(k-\theta)\frac{a}{2}}{\sin(k+\theta)\frac{a}{2}}\right] - k\theta + \frac{1}{4\pi a^2}\int_{e^{i(k+\theta)a}}^{e^{i(k-\theta)a}}\frac{dt}{t}\ln(1-t)\right\}x^3,$$

$$\begin{aligned} F_1(k,x) = -\Bigg\{&\frac{k^2}{8\pi a}\ln[2(\cos(ka)-\cos(\theta a))] \\ &-\frac{ik}{4\pi a^2}\left[\left[\int_0^{e^{i(k-\theta)a}}\frac{dt}{t}\ln(1-t)\right] + \int_0^{e^{i(k+\theta)a}}\frac{dt}{t}\ln(1-t)\right] \\ &+\frac{1}{4\pi a^3}\Bigg[\Bigg[\int_0^{e^{i(k-\theta)a}}\frac{dt}{t}\ln(t)\ln(1-t) + \int_0^{e^{i(k+\theta)a}}\frac{dt}{t}\ln(t)\ln(1-t) \\ &-i(k-\theta)a\int_0^{e^{i(k-\theta)a}}\frac{dt}{t}\ln(1-t) \\ &+i(k+\theta)a\int_0^{e^{i(k+\theta)a}}\frac{dt}{t}\ln(1-t)\Bigg]\Bigg]\Bigg\}(x^3)^2; \end{aligned} \tag{1.5.61}$$

$$x = (\tilde{x}, x^3) \in \mathbb{R}^3, \quad \tilde{x} \in \mathbb{R}^2, \quad x^3 \in \mathbb{R}.$$

Furthermore, ϕ denotes, as usual, any nontrivial solution of

$$(1 + uG_0v)\phi = 0, \qquad \tilde{\phi} = (\operatorname{sgn} V)\phi. \tag{1.5.62}$$

Finally, χ and η are given by (1.5.65) *and* (1.5.66), *respectively. Hence we obtain*

(a) *If $E_0(\theta) = [k_0(\theta)]^2$ is an eigenvalue of $-\Delta_{\alpha,\Lambda_1}(\theta)$, then $E_\varepsilon(\theta) = [k_\varepsilon(\theta)]^2$ is an eigenvalue of $H_{\alpha,\Lambda_1}(\theta)$ which is analytic in ε provided $E_0(\theta) < 0$.*

(b) *If $k_0(\theta)$ is a complex resonance of $-\Delta_{\alpha,\Lambda_1}(\theta)$, i.e., if* $\operatorname{Im} k_0(\theta) < 0$, *then $k_\varepsilon(\theta)$ is a complex resonance of $H_{\varepsilon,\Lambda_1}(\theta)$.*

(c) *If $k_0(\theta)$ is a real resonance of $-\Delta_{\alpha,\Lambda_1}(\theta)$, i.e., if $k_0(\theta) > |\theta|$, then $k_\varepsilon(\theta)$ is a complex resonance of $H_{\varepsilon,\Lambda_1}(\theta)$ if* $\operatorname{Im} k_3(\theta) \neq 0$. *We always have* $\operatorname{Im} k_1(\theta) = 0$, *while* $\operatorname{Im} k_3(\theta) = 0$ *for at most a finite number of the real resonances $k_0(\theta)$ of $-\Delta_{\alpha,\Lambda_1}(\theta)$.*

Proof. The general strategy is the same as in the proofs of Theorems 1.4.9, II.1.3.1, and II.1.3.3. Again one expands the equation

$$[1 + B_\varepsilon(k_\varepsilon(\theta), \theta)]\phi_\varepsilon(\theta) = 0 \tag{1.5.63}$$

in powers of ε where

$$\phi_\varepsilon(\theta) = \phi + \varepsilon\phi'(\theta) + \frac{\varepsilon^2}{2}\phi''(\theta) + O_\theta(\varepsilon^3) \tag{1.5.64}$$

and ϕ satisfies (1.5.62). We then find

$$\begin{aligned} \phi'(\theta) &= \chi + c(\theta)\phi, \\ \chi &= T[\lambda'(0)\phi - \alpha(v, \phi)u], \end{aligned} \tag{1.5.65}$$

where T denotes the reduced resolvent (cf. I.1.2.37), and

$$\begin{aligned} &\phi''(\theta) = \eta + d(\theta)\phi, \\ &\eta = T\bigg\{\lambda''(0)\phi - 2[A_1 + [k_0(\theta)]^2 B_1](v, \phi)u + \frac{[k_0(\theta)]^2}{8\pi}\cdot \\ &\quad \cdot\left[\int_{\mathbb{R}^3} d^3x' |\cdot - x'| v(x')\phi(x')\right]u + \left[\int_{\mathbb{R}^3} dx'\, E_1(k_0(\theta), \cdot - x')v(x')\phi(x')\right]u \\ &\quad - 2\lambda'(0)uG_0 v\chi - 2\alpha(v, \chi)u\bigg\}. \end{aligned} \tag{1.5.66}$$

The constants $c(\theta)$ and $d(\theta)$ do not enter into the formulas for $k_1(\theta)$ and $k_2(\theta)$ and their value is therefore immaterial for (1.5.57). A subtle point occurs when $k_0(\theta)$ is a real resonance of $-\Delta_{\alpha,\Lambda_1}(\theta)$. If $\operatorname{Im} k_\varepsilon(\theta) < 0$, then $[k_\varepsilon(\theta)]^2$ cannot be an eigenvalue of the self-adjoint operator $H_{\varepsilon,\Lambda_1}(\theta)$. From (1.5.59) and (1.5.60) we see that $k_1(\theta)$ is real, while in general $\operatorname{Im} k_2(\theta) \neq 0$, and hence in general the real resonance $k_0(\theta)$ turns into a complex resonance of $H_{\varepsilon,\Lambda_1}(\theta)$. By analyzing the purely imaginary terms in (1.5.60), we find that this can be zero for at most a finite number of $k_0(\theta)$. ■

III.1.6 Monomolecular Layer

The last regular structure to be discussed in this chapter is that of an infinite plane monomolecular layer, which we obtain by replacing the three-dimensional lattice of Sect. 1.4 with a two-dimensional lattice Λ_2, viz.

$$\Lambda_2 = \{n_1 a_1 + n_2 a_2 \in \mathbb{R}^3 | (n_1, n_2) \in \mathbb{Z}^2\}, \tag{1.6.1}$$

where

$$a_j = (0, a_j^2, a_j^3) \in \mathbb{R}^3, \qquad j = 1, 2, \tag{1.6.2}$$

are two independent vectors in $\mathbb{R}^3$. In this way we obtain, as explained in Sect. 1.3, a one-electron model of a monomolecular layer with point interactions. The discussion will proceed very much along the lines of the preceding section. Let Y_2 be the set where we locate the point interaction, i.e.,

$$Y_2 = Y + \Lambda_2 \subset \mathbb{R}^3, \tag{1.6.3}$$

where

$$Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}^3 \tag{1.6.4}$$

is such that

$$y_j = (y_j^1, y_j^2, y_j^3) \in Y, \qquad (y_j^2, y_j^3) \in \hat{\Gamma}_2, \qquad j = 1, \ldots, N. \tag{1.6.5}$$

Here $\hat{\Gamma}_2$ denotes as usual the dual group defined by

$$\hat{\Gamma}_2 = \mathbb{R}^2/\Lambda_2 \tag{1.6.6}$$

when Λ_2 is considered as a subset of $\mathbb{R}^2$ by ignoring the first component. $\hat{\Gamma}_2$ can be identified with

$$\hat{\Gamma}_2 = \{s_1 a_1 + s_2 a_2 \in \mathbb{R}^3 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2\}. \tag{1.6.7}$$

Similarly, the Brillouin zone $\hat{\Lambda}_2$ can be identified with

$$\hat{\Lambda}_2 = \{s_1 b_1 + s_2 b_2 \in \mathbb{R}^3 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2})\}, \tag{1.6.8}$$

where b_1, b_2 provide a basis of the dual lattice Γ_2, i.e.,

$$\begin{aligned} &\Gamma_2 = \{n_1 b_1 + n_2 b_2 \in \mathbb{R}^3 | (n_1, n_2) \in \mathbb{Z}^2\}, \\ &b_j = (0, b_j^2, b_j^3) \in \mathbb{R}^3, \qquad b_j \cdot a_{j'} = 2\pi\delta_{jj'}, \qquad j, j' = 1, 2. \end{aligned} \tag{1.6.9}$$

Whenever convenient, cf. (1.6.5) and (1.6.6), we shall consider $\hat{\Lambda}_2$ and $\hat{\Gamma}_2$ as subsets of $\mathbb{R}^2$ by simply ignoring the first component. Hence we will write, e.g.,

$$(p, \gamma) \in \mathbb{R}^3, \qquad p \in \mathbb{R}, \quad \gamma \in \Gamma_2. \tag{1.6.10}$$

The first goal is to decompose the operators $-\hat{\Delta}_{\alpha, Y+\Lambda_2}$ and $-\Delta_{\alpha, Y+\Lambda_2}$, and for this we first have to decompose the resolvent of the free Hamiltonian, i.e., the resolvent of the Laplacian, in p-space. Let

$$\begin{aligned} &G_k(\theta)\colon L^2(\mathbb{R} \times \Gamma_2) \to L^2(\mathbb{R} \times \Gamma_2) \\ &(G_k(\theta)g)(p, \gamma) = (|(p, \gamma + \theta)|^2 - k^2)^{-1} g(p, \gamma); \\ &k^2 \notin [|\theta|^2, \infty), \quad \operatorname{Im} k \geq 0, \quad g \in L^2(\mathbb{R} \times \Gamma_2), \quad \theta \in \hat{\Lambda}_2, \quad p \in \mathbb{R}, \quad \gamma \in \Gamma_2. \end{aligned} \tag{1.6.11}$$

We also need

$$g_k(x, \theta) = \begin{cases} \dfrac{ik}{4\pi} + e^{i\theta x}\left\{-\dfrac{ik}{4\pi} + \dfrac{1}{8\pi^2}\lim\limits_{\omega\to\infty}\left[\sum\limits_{\substack{\gamma\in\Gamma_2\\|\gamma+\theta|\leq\omega}} \dfrac{|\hat{\Lambda}_2|}{\sqrt{|\gamma+\theta|^2 - k^2}} - 2\pi\omega\right]\right\}, \\ \qquad\qquad x \in \Lambda_2, \\ (4\pi)^{-1}|\hat{\Gamma}_2|^{-1}\lim\limits_{\omega\to\infty}\sum\limits_{\substack{\gamma\in\Gamma_2\\|\gamma+\theta|\leq\omega}} \dfrac{e^{i(\gamma+\theta)\tilde{x}}}{|\gamma+\theta|}\arctan\left(\dfrac{|\gamma+\theta|}{ik}\right), \\ \qquad\qquad x = (0, \tilde{x}) \notin \Lambda_2, \\ \dfrac{1}{2}|\hat{\Gamma}_2|^{-1}\sum\limits_{\gamma\in\Gamma_2} \dfrac{e^{-\sqrt{|\gamma+\theta|^2-k^2}|x^1|}}{\sqrt{|\gamma+\theta|^2 - k^2}} e^{i(\gamma+\theta)\tilde{x}}, \quad x = (x^1, \tilde{x}) \in \mathbb{R}^3, \quad x^1 \neq 0; \\ \qquad\qquad k^2 \notin |\Gamma_2 + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_2, \end{cases} \tag{1.6.12}$$

where

$$|\Gamma_2 + \theta|^2 = \{|\gamma + \theta|^2 \in \mathbb{R} | \gamma \in \Gamma_2\}. \tag{1.6.13}$$

The analogs of the unitary operators $\mathscr{U}$, cf. (1.4.16), and $\tilde{\mathscr{U}}$, cf. (1.4.53), which we denote by $\mathscr{U}_2$ and $\tilde{\mathscr{U}}_2$, respectively, are now defined by

$$\begin{gathered}
\mathscr{U}_2\colon L^2(\mathbb{R}^3) \to L^2(\hat{\Lambda}_2, L^2(\mathbb{R} \times \Gamma_2)) = \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta\, L^2(\mathbb{R} \times \Gamma_2), \\
(\mathscr{U}_2 \hat{f})(\theta, p, \gamma) = \hat{f}((p, \gamma + \theta)), \qquad \theta \in \hat{\Lambda}_2, \quad p \in \mathbb{R}, \quad \gamma \in \Gamma_2, \quad \hat{f} \in L^2(\mathbb{R}^3),
\end{gathered} \tag{1.6.14}$$

and

$$\begin{aligned}
\tilde{\mathscr{U}}_2\colon \mathscr{S}(\mathbb{R}^3) \to L^2(\hat{\Lambda}_2, |\hat{\Lambda}_2|^{-1}\, d^2\theta; L^2(\mathbb{R} \times \hat{\Gamma}_2)) \\
= |\hat{\Lambda}_2|^{-1} \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta\, L^2(\mathbb{R} \times \hat{\Gamma}_2), \\
(\tilde{\mathscr{U}}_2 f)(\theta, p, \nu) = 2\pi \sum_{\lambda \in \Lambda_2} \int_{\mathbb{R}} dx\, f(x, \lambda + \nu) e^{-ipx} e^{-i\lambda\theta}, \\
\theta \in \hat{\Lambda}_2, \quad p \in \mathbb{R}, \quad \nu \in \hat{\Gamma}_2, \quad f \in \mathscr{S}(\mathbb{R}^3).
\end{aligned} \tag{1.6.15}$$

As usual $\tilde{\mathscr{U}}_2$ is extended to $L^2(\mathbb{R}^3)$ by continuity, and the extension is still denoted by $\tilde{\mathscr{U}}_2$.

Theorem 1.6.1. *Let $y_j \in Y$, $(y_j^2, y_j^3) \in \hat{\Gamma}_2$, and $\alpha_j \in \mathbb{R}$, $j = 1, \ldots, N$. Then the operator $-\hat{\Delta}_{\alpha, Y+\Lambda_2}$ in $L^2(\mathbb{R}^3)$ of Theorem* 1.1.1 *with*

$$\alpha_{y_j+\lambda} = \alpha_j, \qquad j = 1, \ldots, N, \quad \alpha = \{\alpha_j\}, \quad \lambda \in \Lambda_2, \tag{1.6.16}$$

satisfies

$$\mathscr{U}_2[-\hat{\Delta}_{\alpha, Y+\Lambda_2}]\mathscr{U}_2^{-1} = \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta [-\hat{\Delta}_{\alpha, \Lambda_2, Y}(\theta)], \tag{1.6.17}$$

where $-\hat{\Delta}_{\alpha, \Lambda_2, Y}(\theta)$ is the self-adjoint operator in $L^2(\mathbb{R} \times \Gamma_2)$ with resolvent

$$\begin{gathered}
(-\hat{\Delta}_{\alpha, \Lambda_2, Y}(\theta) - k^2)^{-1} = G_k(\theta) + \sum_{j, j'=1}^{N} [\Gamma_{\alpha, \Lambda_2, Y}(k, \theta)]_{jj'}^{-1} (F_{-\bar{k}, y_{j'}}(\theta), \cdot) F_{k, y_j}(\theta), \\
k^2 \in \rho(-\Delta_{\alpha, \Lambda_2, Y}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_2, \quad (y_j^2, y_j^3) \in \hat{\Gamma}_2, \\
\alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N,
\end{gathered} \tag{1.6.18}$$

where

$$\Gamma_{\alpha, \Lambda_2, Y}(k, \theta) = [\alpha_j \delta_{jj'} - g_k(y_j - y_{j'}, \theta)]_{j, j'=1}^{N} \tag{1.6.19}$$

and

$$F_{k,y_j}(\theta, p, \gamma) = (2\pi)^{-3/2} \frac{e^{-i(p,\gamma+\theta)y_j}}{|(p, \gamma + \theta)|^2 - k^2},$$

$$k^2 \in \rho(-\hat{\Delta}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_2, \quad p \in \mathbb{R}, \quad \gamma \in \Gamma_2, \quad j = 1, \ldots, N. \tag{1.6.20}$$

If

$$-\Delta_{\alpha, Y+\Lambda_2} = \mathscr{F}^{-1}[-\hat{\Delta}_{\alpha, Y+\Lambda_2}]\mathscr{F}, \tag{1.6.21}$$

then

$$\tilde{\mathscr{U}}_2[-\Delta_{\alpha,Y+\Lambda_2}]\tilde{U}_2^{-1} = |\hat{\Lambda}_2|^{-1} \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta[-\Delta_{\alpha,\Lambda_2,Y}(\theta)], \tag{1.6.22}$$

where $-\Delta_{\alpha,\Lambda_2,Y}(\theta)$ *is the self-adjoint operator in* $L^2(\mathbb{R} \times \hat{\Gamma}_2)$ *with resolvent*

$$(-\Delta_{\alpha,\Lambda_2,Y}(\theta) - k^2)^{-1}$$
$$= g_k(\theta) + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,\Lambda_2,Y}(k, \theta)]_{jj'}^{-1} \overline{(g_k(\cdot - y_{j'}, \theta), \cdot)} g_k(\cdot - y_j, \theta),$$

$$k^2 \in \rho(-\Delta_{\alpha,\Lambda_2,Y}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_2, \quad (y_j^2, y_j^3) \in \hat{\Gamma}_2,$$
$$\alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N. \tag{1.6.23}$$

Here

$$g_k(\theta)\colon L^2(\mathbb{R} \times \hat{\Gamma}_2) \to L^2(\mathbb{R} \times \hat{\Gamma}_2),$$

$$(g_k(\theta)f)(x, v) = \int_{\mathbb{R}} dx' \int_{\hat{\Gamma}_2} d^2v' \, g_k((x - x', v - v'), \theta) f(x', v'),$$

$$k^2 \notin [|\theta|^2, \infty), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}_2, \quad x \in \mathbb{R}, \quad v \in \hat{\Gamma}_2, \quad f \in L^2(\mathbb{R} \times \hat{\Gamma}_2), \tag{1.6.24}$$

and $g_k(x, v)$ *is given by* (1.6.12).

PROOF. Following the proof of Theorem 1.4.3 we get (1.6.17) where $(-\Delta_{\alpha,\Lambda_2,Y}(\theta) - k^2)^{-1}$ equals (1.6.18) with

$$\Gamma_{\alpha,\Lambda_2,Y}(k, \theta) = \left[\left(\alpha_j - \frac{ik}{4\pi}\right)\delta_{jj'} - \sum_{\lambda \in \Lambda_2} \tilde{G}_k(y_j - y_{j'} + \lambda)e^{-i\lambda\theta}\right]_{j,j'=1}^{N}. \tag{1.6.25}$$

By appealing to Lemma 1.6.2, proved after this theorem, we obtain the stated form (1.6.19) of $\Gamma_{\alpha,\Lambda_2,Y}(k, \theta)$. Similarly, the proof of (1.6.22) follows the corresponding proof of Theorem 1.4.3. ■

The next result is the analog of Lemma 1.4.2.

Lemma 1.6.2 (Poisson Summation Formula). *Let $k^2 \in \mathbb{C}$, $\operatorname{Im} k > 0$, $a \in \mathbb{R}^3$, and $\theta \in \hat{\Lambda}_2$. Then*

$$\sum_{\substack{\lambda \in \Lambda_2 \\ \lambda \neq -a}} \frac{e^{ik|\lambda + a|}}{4\pi|\lambda + a|} e^{-i\lambda\theta}$$

$$= \begin{cases} \frac{1}{2}|\hat{\Gamma}_2|^{-1} \sum_{\gamma \in \Gamma_2} \dfrac{e^{-\sqrt{|\gamma+\theta|^2 - k^2}|a^1|}}{\sqrt{|\gamma + \theta|^2 - k^2}} e^{i(\gamma+\theta)\tilde{a}}, \\ \qquad a = (a^1, \tilde{a}) \in \mathbb{R}^3, \quad a^1 \neq 0, \\ (4\pi)^{-1}|\hat{\Gamma}_2|^{-1} \lim\limits_{\omega \to \infty} \sum\limits_{\substack{\gamma \in \Gamma_2 \\ |\gamma+\theta| \leq \omega}} \dfrac{e^{i(\gamma+\theta)\tilde{a}}}{|\gamma + \theta|} \arctan\left(\dfrac{|\gamma + \theta|}{ik}\right), \\ \qquad a = (0, \tilde{a}) \notin \Lambda_2, \\ e^{i\theta a}\left\{-\dfrac{ik}{4\pi} + \dfrac{1}{8\pi^2} \lim\limits_{\omega \to \infty}\left[\sum\limits_{\substack{\gamma \in \Gamma_2 \\ |\gamma+\theta| \leq \omega}} \dfrac{|\hat{\Lambda}_2|}{\sqrt{|\gamma + \theta|^2 - k^2}} - 2\pi\omega\right]\right\}, \\ \qquad a \in \Lambda_2. \end{cases} \tag{1.6.26}$$

PROOF. Consider first $a = 0$. Writing

$$\sum_{\lambda \in \Lambda_2} \tilde{G}_k(\lambda) e^{-i\lambda\theta} = (2\pi)^{-1} \sum_{\substack{\lambda \in \Lambda_2 \\ \lambda \neq 0}} \int_{\mathbb{R}} dp (2\pi)^{-2} \int_{\mathbb{R}^2} d^2\tilde{p} \frac{e^{i\tilde{p}\lambda}}{\tilde{p}^2 + p^2 - k^2} e^{-i\lambda\theta}, \tag{1.6.27}$$

we see that we can exploit the fact that

$$(2\pi)^{-2} \int_{\mathbb{R}^2} d^2\tilde{p} \frac{e^{i\tilde{p}\lambda}}{\tilde{p}^2 + p^2 - k^2} \tag{1.6.28}$$

is the Green's function of the two-dimensional Laplacian at the point λ with energy $p^2 - k^2$. Hence by applying (4.36) we find

$$\begin{aligned} \sum_{\lambda \in \Lambda_2} \tilde{G}_k(\lambda) e^{-i\lambda\theta} &= (2\pi)^{-1} \lim_{\omega \to \infty} \sum_{\substack{\gamma \in \Gamma_2 \\ |\gamma+\theta| \leq \omega}} \int_{\mathbb{R}} dp \left[\frac{|\hat{\Lambda}_2|}{|\gamma + \theta|^2 + p^2 - k^2}\right. \\ &\qquad \left. - \pi \ln(\omega^2 + p^2 - k^2) + \pi \ln(p^2 - k^2)\right] \\ &= \frac{1}{8\pi^2} \lim_{\omega \to \infty} \left[\sum_{\substack{\gamma \in \Gamma_2 \\ |\gamma+\theta| \leq \omega}} \frac{|\hat{\Lambda}_2|}{\sqrt{|\gamma + \theta|^2 - k^2}} - 2\pi\omega\right] - \frac{ik}{4\pi} \end{aligned} \tag{1.6.29}$$

after a short computation. The general case $a \in \Lambda_2$ follows by translation. Assume now that $a = (0, \tilde{a}) \notin \Lambda_2$. By defining

$$f(\omega) = \sum_{\substack{\gamma \in \Gamma_2 \\ |\gamma+\theta| \leq \omega}} \frac{\arctan\left(\dfrac{|\gamma + \theta|}{ik}\right)}{|\gamma + \theta|} e^{i(\gamma+\theta)\tilde{a}}, \qquad \omega > 0, \tag{1.6.30}$$

and

$$F(\eta) = \int_0^\infty e^{-\eta\omega}\, df(\omega), \qquad \eta > 0, \tag{1.6.31}$$

we can follow the analysis used in the proof of Lemma 1.4.2 to obtain the conditional convergence of (1.6.30) as $\omega \to \infty$ and the equality (1.6.26). The last case, when $a = (a^1, \tilde{a}) \in \mathbb{R}^3$, $a^1 \neq 0$, follows directly from [94], Theorem 67 and eq. (19), p. 260. ■

We now turn to the study of spectral properties of $-\hat{\Delta}_{\alpha,\Lambda_2,Y}(\theta)$ and specialize to the case $Y = \{0\}$ from now on.

Theorem 1.6.3. *Let $\alpha \in \mathbb{R}$, $\theta \in \hat{\Lambda}_2$, and define $-\hat{\Delta}_{\alpha,\Lambda_2}(\theta) \equiv -\hat{\Delta}_{\alpha,\Lambda_2,\{0\}}(\theta)$. Then the essential spectrum of $-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)$ is purely absolutely continuous and equals*

$$\sigma_{\mathrm{ess}}(-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)) = \sigma_{\mathrm{ac}}(-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)) = [|\theta|^2, \infty), \qquad \sigma_{\mathrm{sc}}(-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)) = \varnothing, \qquad \theta \in \hat{\Lambda}_2. \tag{1.6.32}$$

In addition, $-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)$ has exactly one simple eigenvalue $E_0^{\alpha,\Lambda_2}(\theta) = [k_0^{\alpha,\Lambda_2}(\theta)]^2 < |\theta|^2$ which is the unique solution of

$$\alpha = g_{k^{\alpha,\Lambda_2}(\theta)}(0, \theta), \qquad \mathrm{Im}\, k^{\alpha,\Lambda_2}(\theta) \geq 0, \quad [k^{\alpha,\Lambda_2}(\theta)]^2 < |\theta|^2. \tag{1.6.33}$$

The corresponding eigenfunction reads

$$\psi_{E_0^{\alpha,\Lambda_2}(\theta)}(\theta, p, \gamma) = [|(p, \gamma + \theta)|^2 - E_0^{\alpha,\Lambda_2}(\theta)]^{-1}, \qquad \theta \in \hat{\Lambda}_2, \quad p \in \mathbb{R}, \quad \gamma \in \Gamma_2. \tag{1.6.34}$$

$E_0^{\alpha,\Lambda_2}(\theta)$ is strictly increasing in α for $\theta \in \hat{\Lambda}_2$.

Proof. Equation (1.6.32) follows as in Theorem 1.5.3. Eigenvalues E are given as solutions of

$$\alpha = g_k(0, \theta), \qquad E = k^2, \qquad \mathrm{Im}\, k \geq 0. \tag{1.6.35}$$

From the explicit form of $g_k(0, \theta)$ we see that $g_k(0, \theta) \to -\infty$ as $k^2 \to -\infty$ and $g_k(0, \theta) \to \infty$ as $k^2 \uparrow |\theta|^2$, and that $g_k(0, \theta)$ is strictly increasing in k^2. ■

Before we turn to the ε-approximation, we give the spectrum of the full Hamiltonian.

Theorem 1.6.4. *Let $\alpha \in \mathbb{R}$ and consider*

$$\mathcal{U}_2[-\hat{\Delta}_{\alpha,\Lambda_2}]\mathcal{U}_2^{-1} = \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta[-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)]. \tag{1.6.36}$$

Then the spectrum of $-\hat{\Delta}_{\alpha,\Lambda_2}$ is absolutely continuous and equals

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda_2}) = \sigma_{\mathrm{ac}}(-\hat{\Delta}_{\alpha,\Lambda_2}) = \begin{cases} [E_0^{\alpha,\Lambda_2}(0), \infty), & \alpha \geq \alpha_{\Lambda_2}, \\ [E_0^{\alpha,\Lambda_2}(0), E_0^{\alpha,\Lambda_2}(\theta_0)] \cup [0, \infty), & \alpha < \alpha_{\Lambda_2}, \end{cases} \tag{1.6.37}$$

with $E_0^{\alpha,\Lambda_2}(0) < 0$ and $E_0^{\alpha,\Lambda_2}(0) < E_0^{\alpha,\Lambda_2}(\theta_0) < 0$ provided $\alpha < \alpha_{\Lambda_2}$ where α_{Λ_2} equals

$$\alpha_{\Lambda_2} = \frac{1}{8\pi^2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma_2 \\ |\gamma+\theta_0|\le\omega}} \frac{|\hat{\Lambda}_2|}{|\gamma+\theta_0|} - 2\pi\omega \right] \tag{1.6.38}$$

and

$$\theta_0 = -(b_1 + b_2)/2. \tag{1.6.39}$$

PROOF. Again the proof is similar to that of Theorem 1.4.5. ■

Finally, we analyze approximations of $-\hat{\Delta}_{\alpha,\Lambda_2}(\theta)$ by Hamiltonians with local scaled, short-range interactions. Let

$$\begin{aligned} &A_\varepsilon(k,\theta)\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}\times\hat{\Gamma}_2), \\ &B_\varepsilon(k,\theta)\colon L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \\ &C_\varepsilon(k,\theta)\colon L^2(\mathbb{R}\times\hat{\Gamma}_2) \to L^2(\mathbb{R}^3), \end{aligned} \tag{1.6.40}$$

be Hilbert–Schmidt operators with integral kernels

$$\begin{aligned} A_\varepsilon(k,\theta,\tilde{x},v,x) &= g_k((\tilde{x},v)-\varepsilon x,\theta)v(x'), \\ B_\varepsilon(k,\theta,x,x') &= \varepsilon\lambda(\varepsilon)u(x)g_k(\varepsilon(x-x'),\theta)v(x'), \\ C_\varepsilon(k,\theta,x,\tilde{x},v) &= \lambda(\varepsilon)u(x)g_k(\varepsilon x-(\tilde{x},v),\theta); \end{aligned}$$

$$\varepsilon\ge 0,\quad k^2\notin|\Gamma_2+\theta|^2,\quad \operatorname{Im} k\ge 0,\quad \theta\in\hat{\Lambda}_2,\quad x,x'\in\mathbb{R}^3,\quad \tilde{x}\in\mathbb{R},\quad v\in\hat{\Gamma}_2. \tag{1.6.41}$$

Theorem 1.6.5. *Let $V\in R$, supp V compact, and $\lambda(\varepsilon) = 1 + \varepsilon\lambda'(0) + o(\varepsilon)$ as $\varepsilon\downarrow 0$ both be real-valued. Then the self-adjoint operator in $L^2(\mathbb{R}^3)$*

$$H_{\varepsilon,\Lambda_2} = -\Delta \dotplus \varepsilon^{-2}\lambda(\varepsilon) \sum_{\lambda\in\Lambda_2} V((\cdot-\lambda)/\varepsilon) \tag{1.6.42}$$

satisfies

$$\tilde{\mathscr{U}}_2 H_{\varepsilon,\Lambda_2} \tilde{\mathscr{U}}_2^{-1} = |\hat{\Lambda}_2|^{-1} \int_{\hat{\Lambda}_2}^{\oplus} d^2\theta\, H_{\varepsilon,\Lambda_2}(\theta), \tag{1.6.43}$$

where $H_{\varepsilon,\Lambda_2}(\theta)$ is the self-adjoint operator in $L^2(\mathbb{R}\times\hat{\Gamma}_2)$ with resolvent

$$\begin{gathered} (H_{\varepsilon,\Lambda_2}(\theta)-k^2)^{-1} = g_k(\theta) - \varepsilon A_\varepsilon(k,\theta)[1+B_\varepsilon(k,\theta)]^{-1}C_\varepsilon(k,\theta), \\ \varepsilon>0,\quad k^2\in\rho(H_{\varepsilon,\Lambda_2}(\theta)),\quad \operatorname{Im} k\ge 0,\quad \theta\in\hat{\Lambda}_2. \end{gathered} \tag{1.6.44}$$

Assume that $\lambda'(0)\ne 0$ if $H = -\Delta \dotplus V$ is in case III *or* IV. *Then $H_{\varepsilon,\Lambda_2}(\theta)$ converges in norm resolvent sense to $-\Delta_{\alpha,\Lambda_2}(\theta)$ as $\varepsilon\downarrow 0$, i.e.,*

$$\operatorname*{n-lim}_{\varepsilon\downarrow 0} (H_{\varepsilon,\Lambda_2}(\theta)-k^2)^{-1} = (-\Delta_{\alpha,\Lambda_2}(\theta)-k^2)^{-1}, \qquad k^2\in\mathbb{C}-\mathbb{R},\quad \theta\in\hat{\Lambda}_2, \tag{1.6.45}$$

where

$$\alpha = \begin{cases} \infty & \textit{in case I}, \\ -\lambda'(0)|(v, \phi)|^{-2} & \textit{in case II}, \\ \infty & \textit{in case III}, \\ -\lambda'(0)\left\{\sum_{j=1}^{N} |(v, \phi_j)|^2\right\}^{-1} & \textit{in case IV}. \end{cases} \tag{1.6.46}$$

PROOF. The proof is similar to that of Theorem 1.4.8. ■

If $\alpha = \infty$, then n-$\lim_{\varepsilon \downarrow 0} (H_{\varepsilon, \Lambda_2}(\theta) - k^2)^{-1} = g_k(\theta)$, the resolvent of the free decomposed Laplacian.

Studying only the unique, simple eigenvalue $E_0^{\alpha, \Lambda_2}(\theta)$ of $-\Delta_{\alpha, \Lambda_2}(\theta)$ below the essential spectrum we get

Theorem 1.6.6. *Let $V \in R$, supp V compact, be real-valued, and let $\lambda(\varepsilon)$, $\lambda(0) = 1$, be real analytic in a neighborhood of zero. Assume $H = -\Delta \dot{+} V$ to be in case* II *and let $\theta \in \hat{\Lambda}_2$. Then $H_{\varepsilon, \Lambda_2}(\theta)$ has a unique simple eigenvalue $E_\varepsilon^{\alpha, \Lambda_2}(\theta) < |\theta|^2$ behaving as*

$$E_\varepsilon^{\alpha, \Lambda_2}(\theta) = E_0^{\alpha, \Lambda_2}(\theta) + \varepsilon E_1^{\alpha, \Lambda_2}(\theta) + O(\varepsilon^2), \tag{1.6.47}$$

where $E_0^{\alpha, \Lambda_2}(\theta)$ is the unique eigenvalue of $-\Delta_{\alpha, \Lambda_2}(\theta)$, $-\Delta_{\alpha, \Lambda_2}(\theta)$ being the norm resolvent limit of $H_{\varepsilon, \Lambda_2}(\theta)$ as $\varepsilon \downarrow 0$, and $E_1^{\alpha, \Lambda_2}(\theta)$ satisfies

$$E_1^{\alpha, \Lambda_2}(\theta) = \tfrac{1}{2} h_{\Lambda_2}(k_0^{\alpha, \Lambda_2}(\theta), \theta)[A_2 + E_0^{\alpha, \Lambda_2}(\theta) B_2], \tag{1.6.48}$$

where

$$h_{\Lambda_2}(k, \theta) = 2|\hat{\Gamma}_2|\left[k \sum_{\gamma \in \Gamma_2} (|\gamma + \theta|^2 - k^2)^{-3/2}\right]^{-1},$$

$$A_2 = \lambda''(0)\frac{(\tilde{\phi}, \phi)}{|(v, \phi)|^2} + \lambda'(0)\frac{(\tilde{\phi}, \chi)}{|(v, \phi)|^2} - \alpha\frac{(v, \chi)}{(v, \phi)} - \lambda'(0)\alpha, \tag{1.6.49}$$

$$B_2 = -\frac{1}{8\pi|(v, \phi)|^2} \int\!\!\int_{\mathbb{R}^6} d^3x\, d^3x'\, \overline{\phi(x)} v(x) |x - x'| v(x') \phi(x'),$$

and χ satisfies (1.5.65).

PROOF. Similar to the proof of Theorem 1.5.6. ■

III.1.7 Bragg Scattering

By *Bragg scattering* we mean the scattering from an infinite half-crystal in three dimensions, more precisely we study the operator $-\Delta_{\alpha, \Lambda_+}$ where

$$\Lambda_+ = \{n_1 a_1 + n_2 a_2 + n_3 a_3 \in \mathbb{R}^3 | (n_1, n_2, n_3) \in \mathbb{Z}^2 \times \mathbb{N}_0\} \tag{1.7.1}$$

with $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$ and a_1, a_2, a_3 is a basis in $\mathbb{R}^3$ and

$$\alpha_\lambda = \alpha \in \mathbb{R}, \qquad \lambda \in \Lambda_+. \tag{1.7.2}$$

While our basic technique in the discussion of the crystal, straight polymer, and monomolecular layer has been the Fourier transform of the full matrix $\Gamma_{\alpha,\Lambda_j}(k)$ in the directions of symmetry, here we will combine this technique with the *Wiener–Hopf* method for inverting a Toeplitz matrix in the direction with "half" symmetry.

Consider a particle coming towards the half-crystal Λ_+ with momentum p', viz.

$$p'b_3 > 0 \tag{1.7.3}$$

where $b_1, b_2, b_3 \in \mathbb{R}^3$ satisfy (cf. Sect. 1.4)

$$a_j b_{j'} = 2\pi\delta_{jj'}, \qquad j \neq j', \;\; j, j' = 1, 2, 3. \tag{1.7.4}$$

Thus b_3 is orthogonal to the surface of Λ_+, pointing into the half-crystal. After being scattered off the half-crystal the particle has momentum p with

$$pb_3 < 0. \tag{1.7.5}$$

Conservation of energy gives

$$p^2 = p'^2 = E = k^2. \tag{1.7.6}$$

Furthermore, *Bragg scattering* imposes that

$$(p - p')\lambda = 0 \,(\mathrm{mod}\, 2\pi), \qquad \lambda \in \Lambda_2, \tag{1.7.7}$$

where

$$\Lambda_2 = \{n_1 a_1 + n_2 a_2 \in \mathbb{R}^3 \mid (n_1, n_2) \in \mathbb{Z}^2\}. \tag{1.7.8}$$

As the next result shows there is only a finite number of reflected momenta p for any given p' satisfying (1.7.5)–(1.7.7).

First, we introduce the necessary new notation. Let

$$\Gamma_2 = \{n_1 b_1 + n_2 b_2 \in \mathbb{R}^3 \mid (n_1, n_2) \in \mathbb{Z}^2\},$$

$$\hat{\Lambda}_2 = \{s_1 b_1 + s_2 b_2 \in \mathbb{R}^3 \mid s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2\}, \tag{1.7.9}$$

$$\tilde{\Lambda} = \{na_3 \in \mathbb{R}^3 \mid n \in \mathbb{N}_0\}, \tag{1.7.10}$$

and for any $q \in \mathbb{R}^3$ we let $q_\parallel$ denote the (not necessarily orthogonal) projection onto the plane orthogonal to a_3, viz.

$$q_\parallel = \frac{1}{2\pi}[(q, a_1)b_1 + (q, a_2)b_2], \qquad q = \sum_{j=1}^{3} q_j b_j, \quad q_\parallel = \sum_{j=1}^{2} q_j b_j. \tag{1.7.11}$$

Theorem 1.7.1. *Let $p' \in \mathbb{R}^3$ and assume* (1.7.3). *Then there is a finite number of $p \in \mathbb{R}^3$ satisfying* (1.7.5)–(1.7.7). *The allowed p can be written in the form*

$$\begin{aligned} p = p_{\gamma_2}(p') = p'_\parallel + \gamma_2 + \{&-|b_3|^{-2}(p'_\parallel + \gamma_2) \\ &- |b_3|^{-1}\sqrt{E - (p'_\parallel + \gamma_2)^2 + [|b_3|^{-1}(p'_\parallel + \gamma_2)b_3]^2}\,\}b_3, \\ &\gamma_2 \in \Gamma_2, \quad E - (p'_\parallel + \gamma_2)^2 + [|b_3|^{-1}(p'_\parallel + \gamma_2)b_3]^2 \geq 0. \end{aligned} \tag{1.7.12}$$

Furthermore,

$$\theta_2 \equiv p'_{\|} \,(\mathrm{mod}\, \Gamma_2) = p_{\|} \,(\mathrm{mod}\, \Gamma_2) \in \hat{\Lambda}_2. \tag{1.7.13}$$

Remark. Observe that $p_0(p')$, i.e., $\gamma_2 = 0$, always satisfies (1.7.5)–(1.7.7) (specular reflection).

PROOF. Starting with condition (1.7.7) we write

$$p - p' = \sum_{j=1}^{3} \beta_j b_j \tag{1.7.14}$$

which inserted into (1.7.7) yields

$$\beta_1, \beta_2 \in \mathbb{Z} \tag{1.7.15}$$

which proves (1.7.13). Thus

$$p = p' + \gamma_2 + \beta_3 b_3, \qquad \gamma_2 \in \Gamma_2. \tag{1.7.16}$$

Squaring we find

$$p'^2 = E = p^2 = (p'_{\|} + \gamma_2)^2 + 2(p'_{\|} + \gamma_2)b_3(\eta + \beta_3) + (\eta + \beta_3)b_3^2, \tag{1.7.17}$$

where

$$p' - p'_{\|} = \eta b_3. \tag{1.7.18}$$

Solving (1.7.17) with respect to $\eta + \beta_3$ we find (1.7.12) using (1.7.5). ∎

Recall from (II.1.5.6) that the off-shell scattering amplitude $f_{\alpha,\Lambda_N}(k, p, p')$ for $(-\Delta, -\Delta_{\alpha,\Lambda_N})$ with

$$\Lambda_N = [-N, N]^3 \cap \Lambda_+ \tag{1.7.19}$$

reads

$$f_{\alpha,\Lambda_N}(k, p, p') = \frac{1}{4\pi} \sum_{\lambda,\lambda' \in \Lambda_N} [\Gamma_{\alpha,\Lambda_N}(k)]^{-1}_{\lambda\lambda'} e^{-ip\lambda} e^{ip'\lambda'},$$

$$\det[\Gamma_{\alpha,\Lambda_N}(k)] \neq 0, \quad \mathrm{Im}\, k \geq 0, \quad p, p' \in \mathbb{C}^3. \tag{1.7.20}$$

The scattering amplitude $f_{\alpha,\Lambda_+}(k, p, p')$ associated with $-\Delta_{\alpha,\Lambda_+}$ will be defined as the weak limit of $f_{\alpha,\Lambda_N}(k, p, p')$ as $N \to \infty$, and our main result will be the computation of its on-shell limit.

Theorem 1.7.2. *Let $f_{\alpha,\Lambda_N}(k, p, p')$, $\mathrm{Im}\, k \geq 0$, $\mathrm{Re}\, k \geq 0$, $p, p' \in \mathbb{C}^3$, be the off-shell scattering amplitude, given by* (1.7.20), *associated with $(-\Delta, -\Delta_{\alpha,\Lambda_N})$ with $\Lambda_N = [-N, N]^3 \cap \Lambda_+$. Then*

$$\lim_{N\to\infty} (g, f_{\alpha,\Lambda_N}(k)f) = (g, f_{\alpha,\Lambda_+}(k)f)$$

$$= \frac{1}{4\pi} \sum_{\lambda,\lambda' \in \tilde{\Lambda}} [\Gamma_{\alpha,\Lambda_+}(k)]^{-1}_{\lambda\lambda'} (e^{-i(\cdot)\lambda'}, f)(g, e^{-i(\cdot)\lambda}),$$

$$f, g \in \mathscr{S}(\mathbb{R}^3), \quad \det[\Gamma_{\alpha,\Lambda_+}(k)] \neq 0, \quad \mathrm{Im}\, k > 0. \tag{1.7.21}$$

Let $p' \in \mathbb{R}^3$ and assume that $p = p_{\tilde{\gamma}_2}(p')$ satisfies (1.7.12) *for some $\tilde{\gamma}_2 \in \Gamma_2$. Then the on-shell scattering amplitude reads*

$$f_{\alpha,\Lambda_+}(|p|, p, p') = -\frac{(p'a_3)|b_3|}{|\hat{\Lambda}|} e^{\pi i(p_3 - p'_3)} \cdot \prod_{\substack{\gamma_2 \in \Gamma_2 \\ \gamma_2 \neq \tilde{\gamma}_2}} \frac{\sin \frac{1}{2}[\beta_{|p|}(\theta_2, \gamma_2) + 2\pi p_3] \sin \frac{1}{2}[\phi_{|p|}(\theta_2, \gamma_2) + 2\pi p'_3]}{\sin \frac{1}{2}[\beta_{|p|}(\theta_2, \gamma_2) + 2\pi p'_3] \sin \frac{1}{2}[\phi_{|p|}(\theta_2, \gamma_2) + 2\pi p_3]}, \tag{1.7.22}$$

where

$$\theta_2 = p_{\|} \ (\mathrm{mod}\ \Gamma_2) = p'_{\|} \ (\mathrm{mod}\ \Gamma_2) \tag{1.7.23}$$

and

$$\beta_k(\theta_2, \gamma_2) = \frac{2\pi}{|b_3|}\sqrt{k^2 - (\theta_2 + \gamma_2)^2 + [|b_3|^{-1}(\theta_2 + \gamma_2)b_3]^2}, \quad \mathrm{Im}\ \beta_k(\theta_2, \gamma_2) \geq 0, \tag{1.7.24}$$

and $\{\phi_k(\theta_2, g_2)|\gamma_2 \in \Gamma_2\}$ solves

$$\Gamma_{\alpha,\Lambda}\left(k, \theta_2 + \frac{\phi_k(\theta_2, \gamma_2)}{2\pi} b_3\right) = 0, \qquad \mathrm{Im}\ \phi_k(\theta_2, \gamma_2) \geq 0. \tag{1.7.25}$$

PROOF. We have

$$(g, f_{\alpha,\Lambda_N}(k)f) = \frac{1}{4\pi} \sum_{\lambda,\lambda' \in \Lambda_N} [\Gamma_{\alpha,\Lambda_+}(k)]^{-1}_{\lambda\lambda'}(e^{-i(\cdot)\lambda'}, f)(g, e^{-i(\cdot)\lambda})$$
$$\xrightarrow[N\to\infty]{} \frac{1}{4\pi} \sum_{\lambda,\lambda' \in \Lambda_+} [\Gamma_{\alpha,\Lambda_+}(k)]^{-1}_{\lambda\lambda'}(e^{-i(\cdot)\lambda'}, f)(g, e^{-i(\cdot)\lambda}),$$
$$\det[\Gamma_{\alpha,\Lambda_+}(k)] \neq 0, \quad \mathrm{Im}\ k > 0, \quad f, g \in \mathscr{S}(\mathbb{R}^3), \tag{1.7.26}$$

since $\{(e^{-i(\cdot)\lambda}, f)\} \in l^2(\Lambda_+)$ when $f \in \mathscr{S}(\mathbb{R}^3)$. Following the proof of Theorem 1.6.1 we infer

$$\frac{1}{4\pi} \sum_{\lambda,\lambda' \in \Lambda_+} [\Gamma_{\alpha,\Lambda_+}(k)]^{-1}_{\lambda\lambda'}(e^{-i(\cdot)\lambda'}, f)(g, e^{-i(\cdot)\lambda})$$
$$= \frac{1}{4\pi} \sum_{\lambda,\lambda' \in \tilde{\Lambda}} \int_{\hat{\Lambda}^2} d^2\theta_2 [\tilde{\Gamma}_{\alpha,\tilde{\Lambda}}(k, \theta_2)]^{-1}_{\lambda\lambda'} e^{-ip_3 b_3 \lambda} e^{ip'_3 b_3 \lambda'} (1, (\mathscr{U}_2 f)(\theta_2))((\mathscr{U}_2 g)(\theta_2), 1),$$
$$\det[\Gamma_{\alpha,\Lambda_+}(k)] \neq 0, \quad \mathrm{Im}\ k > 0, \quad f, g \in \mathscr{S}(\mathbb{R}^3), \tag{1.7.27}$$

with

$$\tilde{\Gamma}_{\alpha,\tilde{\Lambda}}(k, \theta_2) = \left[\left(\alpha - \frac{ik}{4\pi}\right)\delta_{\lambda\lambda'} - \sum_{\lambda_2 \in \Lambda_2} \tilde{G}_k(\lambda - \lambda' + \lambda_2) e^{-i\lambda_2\theta_2}\right]_{\lambda,\lambda' \in \tilde{\Lambda}}, \quad \mathrm{Im}\ k > 0, \tag{1.7.28}$$

and $\mathscr{U}_2$ given by (1.6.14). We use q_3 for the component of a vector $q \in \mathbb{R}^3$ with respect to b_3, cf. (1.7.11). Here the inner products in the first line are in $L^2(\mathbb{R}^3)$, in the second line in $L^2(\mathbb{R} \times \hat{\Gamma}_2)$. To study the on-shell limit we assume

$$p_3, p_3' \in \mathbb{C}, \qquad \operatorname{Im} p_3 < 0, \quad \operatorname{Im} p_3' > 0, \tag{1.7.29}$$

and consider

$$r_{\alpha,\tilde{\Lambda}}(k, \theta_2) = \sum_{\lambda, \lambda' \in \tilde{\Lambda}} [\tilde{\Gamma}_{\alpha,\tilde{\Lambda}}(k, \theta_2)]^{-1}_{\lambda\lambda'} e^{-ip_3 b_3 \lambda} e^{ip_3' b_3 \lambda'}. \tag{1.7.30}$$

Applying the formula [117]

$$\sum_{n,n' \in \mathbb{N}_0} [C]^{-1}_{nn'} s^n t^{n'} = (1 - st)^{-1} \exp\left[\frac{1}{2\pi} \int_{-\pi}^{\pi} dx \frac{(1 - st) \ln [\tilde{C}(x)]}{(s - e^{ix})(t - e^{-ix})}\right], \tag{1.7.31}$$

where

$$C = [C_{nn'}]_{n,n' \in \mathbb{N}_0}, \qquad C_{nn'} = C_{n-n'}, \quad n, n' \in \mathbb{N}_0, \tag{1.7.32}$$

and

$$s, t \in \mathbb{C}, \qquad |s|, |t| < 1 \tag{1.7.33}$$

and

$$\tilde{C}(x) = \sum_{n \in \mathbb{Z}} c_n e^{-inx}, \qquad c_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx\, \tilde{C}(x) e^{inx} \tag{1.7.34}$$

to (1.7.30) we find

$$\begin{aligned} \tilde{\Gamma}_{\alpha,\tilde{\Lambda}}(k, \theta_2) &= [1 - e^{-2\pi i(p_3 - p_3')}]^{-1} \cdot \\ &\cdot \exp\left\{\frac{1}{2\pi} \int_{-\pi}^{\pi} dx \frac{[1 - e^{-2\pi i(p_3 - p_3')}] \ln\left[\Gamma_{\alpha,\Lambda}\left(k, \theta_2 + \frac{x}{2\pi} b_3\right)\right]}{(e^{-2\pi i p_3} - e^{ix})(e^{2\pi i p_3'} - e^{-ix})}\right. \end{aligned} \tag{1.7.35}$$

since

$$\begin{aligned} \tilde{C}(x) &= \alpha - \frac{ik}{4\pi} - \sum_{n \in \mathbb{Z}} \sum_{\lambda_2 \in \Lambda_2} \tilde{G}_k(na_3 + \lambda) e^{-i\lambda_2 \theta_2} e^{-inx} \\ &= \alpha - \frac{ik}{4\pi} - \sum_{\lambda \in \Lambda} \tilde{G}_k(\lambda) e^{-i(\theta_2 + (x/2\pi) b_3)\lambda} \\ &= \Gamma_{\alpha,\Lambda}\left(k, \theta_2 + \frac{x}{2\pi} b_3\right), \qquad \operatorname{Im} k > 0. \end{aligned} \tag{1.7.36}$$

Let (cf. the following Lemma 1.7.3)

$$\begin{aligned} &\Gamma_\omega(k, \theta_2, z) \\ &= \frac{|\hat{\Lambda}|}{\pi |b_3|^2} \left\{ \sum_{\substack{\gamma_2 \in \Gamma_2 \\ |\gamma_2| \le \omega}} \frac{\sin[\beta_k(\theta_2, \gamma_2)]}{\beta_k(\theta_2, \gamma_2)} \frac{1}{z + z^{-1} - 2\cos[\beta_k(\theta_2, \gamma_2)]} + \frac{|b_3|}{4\pi |\gamma_2|} \right\} + \tilde{\alpha} \end{aligned} \tag{1.7.37}$$

and

$$\Gamma(k, \theta_2, z) = \lim_{\omega \to \infty} \Gamma_\omega(k, \theta_2, z), \qquad z \in \mathbb{C} - \{0\}, \tag{1.7.38}$$

where $\beta_k(\theta_2, \gamma_2)$ is given by (1.7.24). Then

$$r_{\alpha,\tilde{\Lambda}}(k, \theta_2)$$
$$= [1 - e^{-2\pi i(p_3 - p_3')}]^{-1} \exp\left\{\frac{1}{2\pi i}\int_{|z|=1} dz \frac{[1 - e^{-2\pi i(p_3 - p_3')}]\ln[\Gamma(k, \theta_2, z)]}{(e^{-2\pi i p_3} - z)(e^{2\pi i p_3'} - z^{-1})z}\right\}$$
$$= [1 - e^{-2\pi i(p_3 - p_3')}]^{-1} \cdot$$
$$\cdot \lim_{\omega\to\infty} \exp\left\{-\frac{1}{2\pi i}\int_{|z|=1} dz \frac{(e^{-2\pi i p_3} - e^{-2\pi i p_3'})\ln[\Gamma_\omega(k, \theta_2, z)]}{(e^{-2\pi i p_3} - z)(z - e^{-2\pi i p_3'})}\right\}. \tag{1.7.39}$$

Consider now the integral

$$I_\omega = -\frac{1}{2\pi i}\int_{|z|=1} \frac{(e^{-2\pi i p_3} - e^{-2\pi i p_3'})\ln[\Gamma_\omega(k, \theta_2, z)]}{(e^{-2\pi i p_3} - z)(z - e^{-2\pi i p_3'})}. \tag{1.7.40}$$

Since $\Gamma_\omega(k, \theta_2, z)$ is a meromorphic function on the Riemann sphere $\mathbb{C} \cup \{\infty\}$, it has an equal number of poles and zeros. Thus $\ln[\Gamma_\omega(k, \theta_2, z)]$ has cuts connecting every pair of poles and zeros. The poles of $\Gamma(k, \theta_2, z)$ are given as solutions $z^{\pm}_{\gamma_2}(k, \theta_2)$ of

$$z^{\pm}_{\gamma_2}(k, \theta_2) + [z^{\pm}_{\gamma_2}(k, \theta_2)]^{-1} = 2\cos[\beta_k(\theta_2, \gamma_2)]. \tag{1.7.41}$$

Define $z^{\pm}_{\omega}(k, \theta_2, \rho)$ as the solutions of

$$z^{\pm}_{\omega}(k, \theta_2, \rho) + [z^{\pm}_{\omega}(k, \theta_2, \rho)]^{-1} = \eta_\omega(k, \theta_2, \rho), \tag{1.7.42}$$

where $\eta_w(k, \theta_2, \rho)$ solves

$$F_\omega(k, \theta_2, \eta_\omega(k, \theta_2, \rho)) = \rho \tag{1.7.43}$$

with

$$F_\omega(k, \theta_2, \xi) = \frac{|\tilde{\Lambda}|}{2\pi|b_3|^2} \sum_{\substack{\gamma_2\in\Gamma_2\\ |\gamma_2|\le\omega}} \left\{\frac{\sin[\beta_k(\theta_2, \gamma_2)]}{\beta_k(\theta_2, \gamma_2)} \frac{1}{\xi - \cos[\beta_k(\theta_2, \gamma_2)]} + \frac{|b_3|}{2\pi|\gamma_2|}\right\} + \tilde{\alpha},$$
$$F(k, \theta_2, \xi) = \lim_{\omega\to\infty} F_\omega(k, \theta_2, \xi). \tag{1.7.44}$$

Hence

$$\Gamma_\omega(k, \theta_2, z) = F_\omega(k, \theta_2, \tfrac{1}{2}(z + z^{-1})). \tag{1.7.45}$$

$F(k, \theta_2, \cdot)$ is a meromorphic function on $\mathbb{C}$ with poles at $\{2\cos[\beta_k(\theta_2, \gamma_2)] | \gamma_2 \in \Gamma_2\}$. If $\beta_k(\theta_2, \gamma_2) \in \mathbb{R}$, then $\cos[\beta_k(\theta_2, \gamma_2)] \in [-1, 1]$, and if $i\beta_k(\theta_2, \gamma_2) < 0$, then $\cos[\beta_k(\theta_2, \gamma_2)] > 1$. Let $\eta(k, \theta_2, \rho)$ be the solution of

$$F(k, \theta_2, \eta(k, \theta_2, \rho)) = \rho. \tag{1.7.46}$$

As $\rho \to \infty$, $\eta(k, \theta_2, \rho) \to \cos[\beta_k(\theta_2, \gamma_2)]$ for some $\gamma_2 \in \Gamma_2$, and we denote this solution of (1.7.46) by $\eta_{\gamma_2}(k, \theta_2, \rho)$. Similarly, we denote by $\eta_{\omega,\gamma_2}(k, \theta_2, \rho)$ the solution of $F_\omega(k, \theta_2, \eta_{\omega,\gamma_2}(k, \theta_2, \rho)) = \rho$ such that $\eta_{\omega,\gamma_2}(k, \theta_2, \rho) \to \cos[\beta_k(\theta_2, \gamma_2)]$ as $\rho \to \infty$. With $\eta_{\omega,\gamma_2}(k, \theta_2, \rho)$ we can then associate $z^{\pm}_{\omega,\gamma_2}(k, \theta_2, \rho)$ using (1.7.42), and $z^{\pm}_{\omega,\gamma_2}(k, \theta_2) \to z^{\pm}_{\gamma_2}(k, \theta_2)$ as $\omega \to \infty$. Ordering the set $\{\cos[\beta_k(\theta_2, \gamma_2)] | \gamma_2 \in \Gamma_2\}$, i.e.,

$$-1 \le \cos[\beta_k(\theta_2, \gamma_2^1)] \le \cdots \le \cos[\beta_k(\theta_2, \gamma_2^{m-1})] \le 1 \le \cos[\beta_k(\theta_2, \gamma_2^m)] \le \cdots, \tag{1.7.47}$$

we have

$$\cos[\beta_k(\theta_2, \gamma_2^{j-1})] \le \eta_{\gamma_2^{j-1}}(k, \theta_2, \rho) \le \cos[\beta_k(\theta_2, \gamma_2^{j})], \qquad j > m. \tag{1.7.48}$$

From the above analysis we infer that we can parametrize the cuts of $\ln[\Gamma_\omega(k, \theta_2, z)]$ by

$$C^{\pm}_{\omega,\gamma_2}(k, \theta_2) = \{z^{\pm}_{\omega,\gamma_2}(k, \theta_2, \rho) | \rho \in [0, \infty)\}. \tag{1.7.49}$$

$\Gamma(k, \theta_2 + (x/2\pi)b_3)$ has no zeros or poles in a uniform strip around the real axis, the width of which depends on $\operatorname{Im} k$. This implies that for ω sufficiently large $|z^{\pm}_{\omega,\gamma_2}(\rho)| \ne 1$, $\gamma_2 \in \Gamma_2$. Since

$$z^{\pm}_{\omega,\gamma_2}(\rho) \xrightarrow[\rho\to\infty]{} e^{\pm i\beta_k(\theta_2,\gamma_2)} \tag{1.7.50}$$

we have

$$C^{+}_{\omega,\gamma_2} \subset \{z \in \mathbb{C} \,|\, |z| < 1\}, \qquad C^{-}_{\omega,\gamma_2} \subset \{z \in \mathbb{C} \,|\, |z| > 1\}, \qquad \gamma_2 \in \Gamma_2. \tag{1.7.51}$$

Hence

$$\begin{aligned}
I_\omega &= -\sum_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \int_{C^{+}_{\omega,\gamma_2}} dz \frac{(e^{-2\pi i p_3} - e^{-2\pi i p_3'})}{(e^{-2\pi i p_3} - z)(z - e^{-2\pi i p_3'})} - \ln[\Gamma_\omega(k, \theta_2, e^{-2\pi i p_3})] \\
&= -\sum_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \int_{C^{+}_{\omega,\gamma_2}} dz \left[\frac{1}{e^{-2\pi i p_3} - z} + \frac{1}{z - e^{-2\pi i p_3'}}\right] - \ln[\Gamma_\omega(k, \theta_2, e^{-2\pi i p_3})] \\
&= \sum_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \ln\left\{\frac{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3]\sin\frac{1}{2}[z^{\pm}_{\omega,\gamma_2}(k,\theta_2,0) + 2\pi p_3']}{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3']\sin\frac{1}{2}[z^{\pm}_{\omega,\gamma_2}(k,\theta_2,0) + 2\pi p_3]}\right\} \\
&\quad - \ln[\Gamma_\omega(k, \theta_2, e^{-2\pi i p_3})],
\end{aligned} \tag{1.7.52}$$

which implies that

$$\begin{aligned}
r_{\alpha,\tilde{\Lambda}}(k, \theta_2) &= [1 - e^{-2\pi i(p_3 - p_3')}]^{-1}[\Gamma(k, \theta_2, e^{-2\pi i p_3})]^{-1} \cdot \\
&\quad \cdot \lim_{\omega\to\infty} \prod_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \frac{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3]\sin\frac{1}{2}[z^{+}_{\omega,\gamma_2}(k,\theta_2,0) + 2\pi p_3']}{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3']\sin\frac{1}{2}[z^{+}_{\omega,\gamma_2}(k,\theta_2,0) + 2\pi p_3]}.
\end{aligned} \tag{1.7.53}$$

Furthermore, we have

$$z^{+}_{\omega,\gamma_2}(k, \theta_2, 0) \xrightarrow[\omega\to\infty]{} \phi_k(\theta_2, \gamma_2), \tag{1.7.54}$$

where $\{\phi_k(\theta_2, \gamma_2) | \gamma_2 \in \Gamma_2\}$ solves

$$\Gamma_{\alpha,\Lambda}\left(k, \theta_2 + \frac{\phi_k(\theta_2,\gamma_2)}{2\pi} b_3\right) = 0, \qquad \operatorname{Im}\phi_k(\theta_2, \gamma_2) \ge 0. \tag{1.7.55}$$

From the proof of Lemma 1.7.3 we infer that

$$\begin{aligned}
-i\beta_k(\theta_2, \gamma_2) &\underset{|\gamma_2|\to\infty}{=} c|\gamma_2| + O(1), \qquad c > 0, \\
-iz^{+}_{\omega,\gamma_2}(k, \theta_2, 0) &\underset{|\gamma_2|\to\infty}{=} c|\gamma_2| + O(1), \qquad c > 0, \quad \gamma_2 \in \Gamma_2,
\end{aligned} \tag{1.7.56}$$

implying that the product converges uniformly as $\omega \to \infty$ and that the convergence is uniform in p_3, p_3'. Taking first the limit $\omega \to \infty$ term-by-term in (1.7.53) we find

$$r_{\alpha,\tilde{\Lambda}}(k, \theta_2) = [1 - e^{-2\pi i(p_3 - p_3')}]^{-1}[\Gamma(k, \theta_2, e^{-2\pi i p_3})]^{-1} \cdot \\ \cdot \lim_{\omega\to\infty} \prod_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \frac{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3]\sin\frac{1}{2}[\phi_k(\theta_2,\gamma_2) + 2\pi p_3']}{\sin\frac{1}{2}[\beta_k(\theta_2,\gamma_2) + 2\pi p_3']\sin\frac{1}{2}[\phi_k(\theta_2,\gamma_2) + 2\pi p_3]}. \quad (1.7.57)$$

As $\operatorname{Im} p_3$, $\operatorname{Im} p_3' \to 0$, we get

$$[\Gamma(k, \theta_2, e^{-2\pi i p_3})]^{-1} \to 0 \quad (1.7.58)$$

and

$$\sin\tfrac{1}{2}[\beta_k(\theta_2, \tilde{\gamma}_2) + 2\pi p_3'] \to 0, \quad (1.7.59)$$

where $p = p_{\tilde{\gamma}_2}(p')$ for some $\tilde{\gamma}_2 \in \Gamma_2$. However, their ratio has a nontrivial limit. A short computation then gives (1.7.22). ∎

We see that formula (1.7.22) expresses the on-shell scattering amplitude as an infinite product of terms depending on the incoming and reflected momenta, respectively. The term depending on the incoming momentum (which equals the inverse of the corresponding term of the reflected momentum) coincides with the ratio of two terms, one as if the crystal filled all of $\mathbb{R}^3$ and one as if there was no crystal.

It remains to state

Lemma 1.7.3. *Let $k \in \mathbb{C}$, $\operatorname{Im} k > 0$. Then*

$$\Gamma_{\alpha,\Lambda}(k, p) = \frac{|\hat{\Lambda}|}{2\pi|b_3|^2} \cdot \\ \cdot \lim_{\omega\to\infty} \sum_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \left\{ \frac{\sin[\beta_k(\theta_2,\gamma_2)]}{\beta_k(\theta_2,\gamma_2)\{\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]\}} \\ + \frac{|b_3|}{2\pi|\gamma_2|}\right\} + \tilde{\alpha}, \quad (1.7.60)$$

where

$$p = \gamma_2 + \theta_2 + (x + n)b_3, \\ \gamma_2 \in \Gamma_2, \quad n \in \mathbb{Z}, \quad \theta_2 = p_\parallel \,(\mathrm{mod}\, \Gamma_2) \in \hat{\Lambda}_2, \quad x \in \mathbb{C}, \quad (1.7.61)$$

and $\tilde{\alpha}$ is independent of k, θ_2, and x.

PROOF. Let $G(x)$ denote the left-hand side of (1.7.60) considered as a function of x alone, and let

$$p' = \gamma_2 + \theta_2 + (x' + n)b_3. \quad (1.7.62)$$

Then

$$
\begin{aligned}
&G(x) - G(x') \\
&\quad = (2\pi)^{-3}|\hat{\Lambda}| \sum_{\gamma\in\Gamma} \left[\frac{1}{(\gamma+p)^2 - k^2} - \frac{1}{(\gamma+p')^2 - k^2}\right] \\
&\quad = (2\pi)^{-3}|\hat{\Lambda}| \sum_{\substack{\gamma\in\Gamma \\ \gamma=\gamma_2+nb_3}} \left[\frac{1}{[\theta_2+\gamma_2+(x+n)b_3]^2 - k^2} \right. \\
&\qquad\qquad \left. - \frac{1}{[\theta_2'+\gamma_2+(x'+n)b_3]^2 - k^2}\right] \\
&\quad = (2\pi)^{-3}|b_3|^{-2}|\hat{\Lambda}| \cdot \\
&\qquad \cdot \sum_{\gamma_2\in\Gamma_2} \sum_{n\in\mathbb{Z}} \left[\frac{1}{(x+n)^2 + 2|b_3|^{-2}(\theta_2+\gamma_2)b_3(x+n) + |b_3|^{-2}[(\theta_2+\gamma_2)^2 - k^2]} \right. \\
&\qquad \left. - \frac{1}{(x'+n)^2 + 2|b_3|^{-2}(\theta_2+\gamma_2)b_3(x'+n) + |b_3|^{-2}[(\theta_2+\gamma_2)^2 - k^2]}\right] \\
&\quad = (2\pi)^{-1}|b_3|^{-2}|\hat{\Lambda}| \sum_{\gamma_2\in\Gamma_2} \frac{\sin[\beta_k(\theta_2,\gamma_2)]}{\beta_k(\theta_2,\gamma_2)} \cdot \\
&\qquad \cdot \left\{\frac{1}{\cos[\beta_k(\theta_2,\gamma_2)] - \cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3]} \right. \\
&\qquad \left. - \frac{1}{\cos[\beta_k(\theta_2,\gamma_2)] - \cos 2\pi[x' + |b_3|^{-2}(\theta_2+\gamma_2)b_3]}\right\},
\end{aligned}
\tag{1.7.63}
$$

where $\beta_k(\theta_2, \gamma_2)$ is given by (1.7.24). Define now

$$
d_{\gamma_2}(x) = \frac{\sin[\beta_k(\theta_2,\gamma_2)]}{\beta_k(\theta_2,\gamma_2)} \frac{1}{\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} + \frac{|b_3|}{2\pi|\gamma_2|}.
\tag{1.7.64}
$$

Then

$$
\begin{aligned}
d_{\gamma_2}(x) &= [\beta_k(\theta_2,\gamma_2)]^{-1}\left\{\frac{\sin[\beta_k(\theta_2,\gamma_2)]}{\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} + i\right\} \\
&\quad - i\beta_k(\theta_2,\gamma_2)^{-1} + \frac{|b_3|}{2\pi|\gamma_2|} \\
&= [\beta_k(\theta_2,\gamma_2)]^{-1} \cdot \\
&\quad \cdot \frac{i\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] + \sin[\beta_k(\theta_2,\gamma_2)] - i\cos[\beta_k(\theta_2,\gamma_2)]}{\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} \\
&\quad - \frac{i|\gamma_2| - (2\pi)^{-1}|b_3|\beta_k(\theta_2,\gamma_2)}{\beta_k(\theta_2,\gamma_2)|\gamma_2|} \\
&= i[\beta_k(\theta_2,\gamma_2)]^{-1}\frac{2\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - e^{i\beta_k(\theta_2,\gamma_2)}}{2\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} \\
&\quad + i\frac{2\theta_2\gamma_2 - |b_3|^{-2}\gamma_2 b_3}{2\beta_k(\theta_2,\gamma_2)|\gamma_2|^2} + O(|\gamma_2|^{-3})
\end{aligned}
\tag{1.7.65}
$$

since

$$\beta_k(\theta_2, \gamma_2) = \frac{2\pi i}{|b_3|}\left[|\gamma_2| - \frac{\theta_2\gamma_2}{|\gamma_2|} + \frac{(\theta_2 b_3)(\gamma_2 b_3)}{2|b_3|^2|\gamma_2|}\right] + O(|\gamma_2|^{-1}). \tag{1.7.66}$$

Let B_ω be the circle in the plane spanned by b_1 and b_2 with radius ω centered at the origin. Then

$$\sum_{\gamma_2\in\Gamma_2\cap B_\omega} d_{\gamma_2}(x) = \sum_{\gamma_2\in\Gamma_2\cap B_\omega}\Bigg\{i[\beta_k(\theta_2,\gamma_2)]^{-1}\cdot \frac{2\cos 2\pi[x + |b_3|^{-2}(\theta_2+\gamma_2)b_3] - e^{i\beta_k(\theta_2,\gamma_2)}}{2\cos 2\pi[x+|b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} + O(|\gamma_2|^{-3})\Bigg\} \tag{1.7.67}$$

since $\Gamma_2 \cap B_\omega$ is invariant with respect to $\gamma_2 \to -\gamma_2$, and $\theta_2\gamma_2$ and $\gamma_2 b_3$ are uneven with respect to this transformation. Hence we infer that

$$\lim_{\omega\to\infty}\sum_{\gamma_2\in\Gamma_2\cap B_\omega} d_{\gamma_2}(x) \tag{1.7.68}$$

exists, and finally that

$$G(x) = (2\pi)^{-1}|b_3|^{-2}|\hat{\Lambda}| \lim_{\omega\to\infty}\left\{\sum_{\substack{\gamma_2\in\Gamma_2\\|\gamma_2|\le\omega}} \frac{\sin[\beta_k(\theta_2,\gamma_2)]}{\beta_k(\theta_2,\gamma_2)}\cdot \frac{1}{\cos 2\pi[x+|b_3|^{-2}(\theta_2+\gamma_2)b_3] - \cos[\beta_k(\theta_2,\gamma_2)]} - \frac{|b_3|}{2\pi|\gamma_2|}\right\} + \tilde{\alpha} - \alpha, \tag{1.7.69}$$

where $\tilde{\alpha}$ is independent of k, θ_2, and x. ■

III.1.8 Fermi Surfaces

The concept of the Fermi surface, which is of vital importance in solid state physics, allows us to relate several of the topics so far discussed in this chapter.

Consider an infinite, perfect crystal and assume that we remove all the electrons from the crystal, and that we intend to put them back one by one. In addition, suppose that we have absolute temperature $T = 0$ so that the electrons go into states with as low energy as possible. The electrons, obeying Fermi–Dirac statistics, satisfy the Pauli principle. By taking into consideration the spin, this means that at most two electrons can have the same energy. Hence the first two electrons occupy a state which corresponds to the bottom of the ground state band, while the next two electrons go into a state with a slightly higher energy and so on. When all the electrons are put back, we have reached some energy E_F, the *Fermi energy*.

To model this we consider, as explained in Sect. 1.3, the one electron model with point interactions, i.e., the operator $-\Delta_{\alpha,\Lambda}$ where Λ is the Bravais lattice.

Recall from Theorem 1.4.4 that

$$\sigma(-\Delta_{\alpha,\Lambda}) = [E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)] \cup [E_1^{\alpha,\Lambda}, \infty) \tag{1.8.1}$$

with $E_0^{\alpha,\Lambda}(\theta_0) < 0$ as long as $\alpha < \alpha_{0,\Lambda}$.

In terms of the *density of states*, formally defined by, e.g., ([161], p. 7)

$$\rho^{\alpha,\Lambda}(E) = \frac{i}{2\pi}\operatorname{Tr}[(-\Delta_{\alpha,\Lambda} - E - i0)^{-1} - (-\Delta_{\alpha,\Lambda} - E + i0)^{-1}] \tag{1.8.2}$$

the Fermi energy can then be defined by

$$\rho^{\alpha,\Lambda}(E_{\mathrm{F}}) = N/2 \tag{1.8.3}$$

where N is the number of electrons per nucleus. (The factor 2 comes from the Pauli principle.)

However, the three-dimensional crystal does not seem to allow a simple expression for the density of states, so we will not give any explicit formula for (1.8.2) (see, however, [215]). (In one dimension one can compute (1.8.2) explicitly, see Sect. 2.3.) The *Fermi surface* is then defined to be the set

$$F_{\alpha,\Lambda}(E_{\mathrm{F}}) = \{\theta \in \hat{\Lambda} \mid \exists \gamma \in \Gamma\colon E_\gamma^{\alpha,\Lambda}(\theta) = E_{\mathrm{F}}\}. \tag{1.8.4}$$

Within the framework of the one-electron model of a solid, we can explain some of the corresponding conductivity properties. Namely, if E_{F} is at the bottom of a gap between the valence (filled) band and the conduction (empty) band, then there is a certain amount of energy needed to excite some electrons. Hence we have an insulator. If E_{F} is sufficiently far away from the upper end of the valence band, one has a metal. Similarly, in the intermediate cases where either the gap is small or E_{F} is fairly close to the end of the valence band, the metal/insulator distinction becomes less sharp and one gets semiconductors or semimetals.

Returning to the Fermi surface we can state the following

Theorem 1.8.1. *Let $\alpha \in \mathbb{R}$ and Λ be a Bravais lattice. Then the Fermi surface for the operator $-\Delta_{\alpha,\Lambda}$ is the set*

$$F_{\alpha,\Lambda}(E_{\mathrm{F}}) = \left\{ \theta \in \hat{\Lambda} \mid 4\pi\alpha = -\kappa_{\mathrm{F}} + \sum_{\substack{\lambda\in\Lambda\\ \lambda\neq 0}} \frac{e^{-\kappa_{\mathrm{F}}|\lambda|}}{|\lambda|}\cos(\theta\lambda) \right\}, \tag{1.8.5}$$

where $E_{\mathrm{F}} = -\kappa_{\mathrm{F}}^2$, $\kappa_{\mathrm{F}} > 0$, is the Fermi energy.

Proof. Equation (1.8.5) follows immediately from (1.8.4) and formula (1.4.38) used in Theorem 1.4.1. ■

The actual computation of a Fermi surface in solid state physics is usually done by combining theory and experiment (see, e.g., [126]). By performing various experiments one can measure, e.g., the diameters for different cross-sections of the Fermi surface. In combination with a parameter-fitting approach, the Fermi surface for most of the simpler metals has been determined to a high degree of accuracy. What we do here is a somewhat different approach: After having chosen the potential, we do not introduce any other approximations.

With the aid of a computer we have illustrated the Fermi surface for various values of E_F, α, and Λ, see Figures 7–33.

A few words are appropriate to explain the illustrations: The Fermi surface as defined by (1.8.4) is a multivalued surface, or if one extends it periodically to $\mathbb{R}^3$ (i.e., replace $\hat{\Lambda}$ by $\mathbb{R}^3$) an infinitely many-valued surface, in the following sense. By solving for one of the components θ_j of $\theta = (\theta_1, \theta_2, \theta_3)$ in terms of the remaining components, we obtain a multivalued (infinitely many-valued) function. In the figures we have only illustrated a single-valued function, more precisely we have illustrated the part of the surface nearest to the origin with $\theta_3 \geq 0$.

The edges of the surface of the Brillouin zone are also included in the illustrations.

Strictly horizontal or vertical parts of the illustrations are not part of the Fermi surface.

Finally, contour plots are also provided for some of the illustrations.

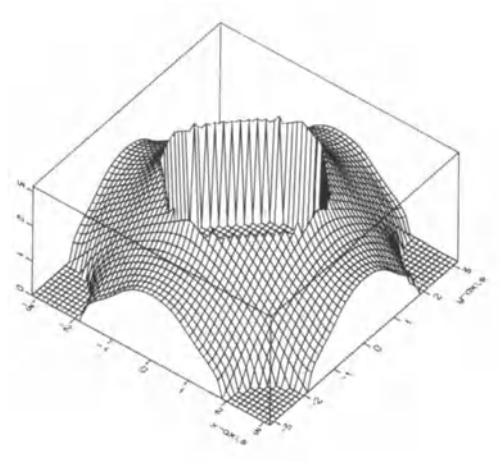


Figure 7 The simplest Fermi surface we include here is for a simple cubic crystal (SC or cubic P) with $E = -1$ and $\alpha = 0.12$ and $a = b = c = 1$ (for notation concerning the lattices, see [290]) inside the upper half of its Brillouin zone. Completely vertical or horizontal parts of the illustration are not parts of the Fermi surface.

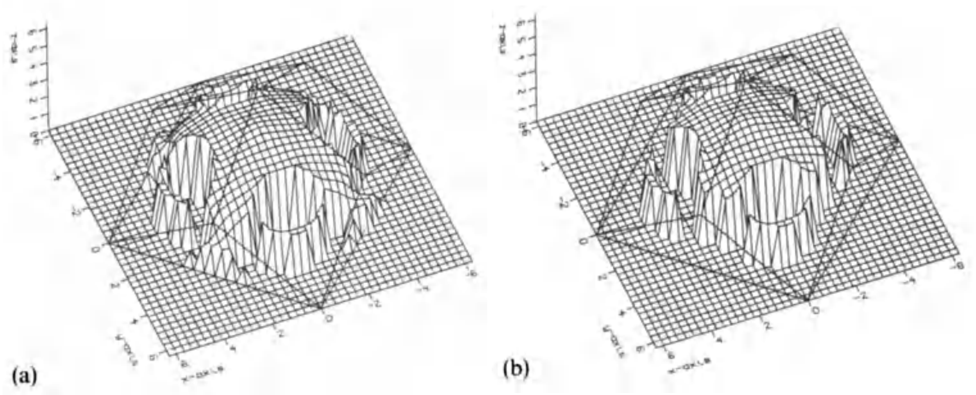


Figure 8 (a) and (b) The Fermi surface of a body centered crystal (BBC or cubic I) with $E = -1$ and $\alpha = -0.14$ inside the upper half of its Brillouin zone. The total surface within the upper half of the Brillouin zone is the union of the two surfaces depicted above.

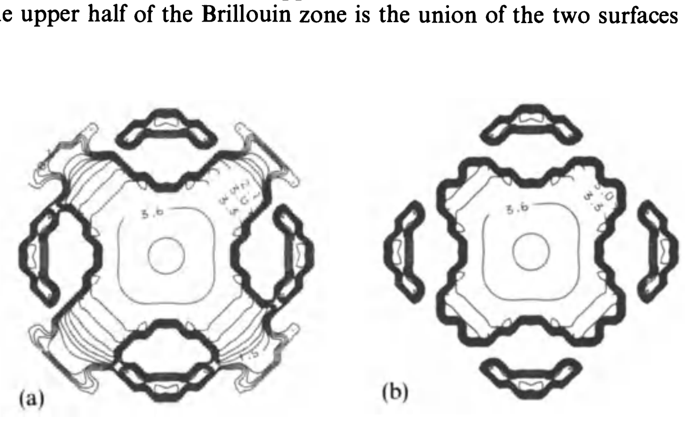


Figure 9 (a) and (b) A contour plot of Figure 8 (a) and (b).

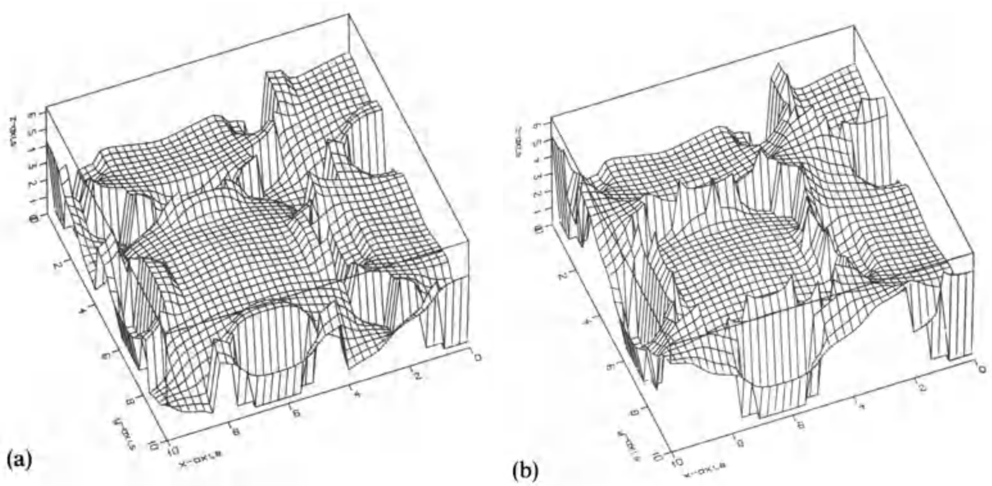


Figure 10 (a) and (b) The Fermi surface of Figure 8 (a) and (b) extended periodically. Again it is difficult to vizualize the total surface in the sense that the total Fermi surface is the union of the two surfaces above extended periodically in the positive and negative z-direction.

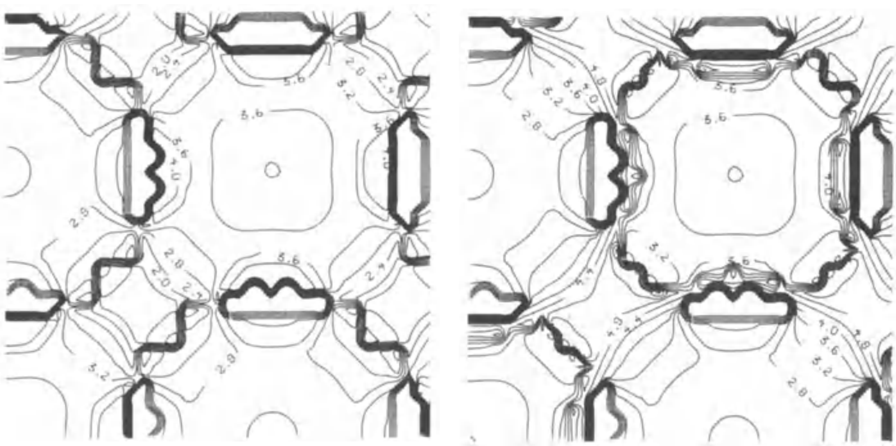


Figure 11 (a) and (b) A contour plot of Figure 10 (a) and (b).

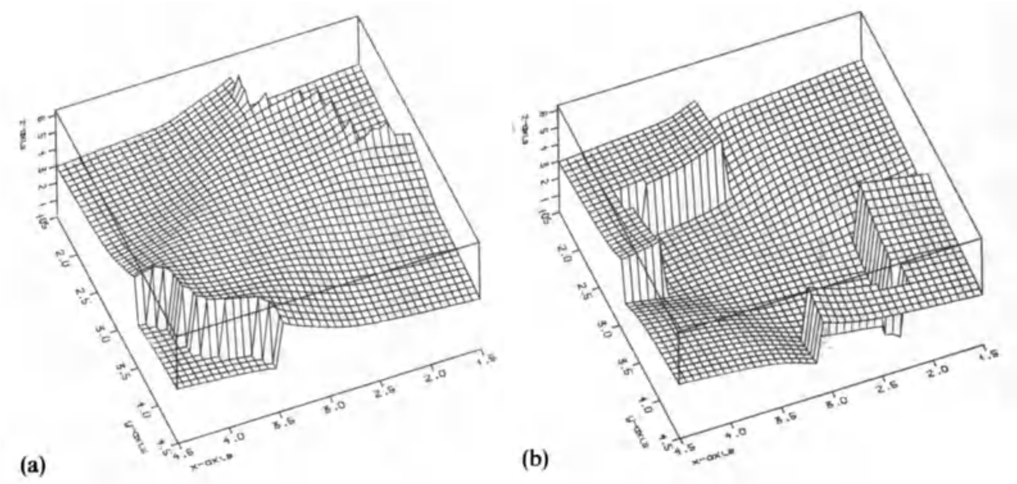


Figure 12 (a) and (b) A magnification of part of the surface in Figure 10 (a) and (b).

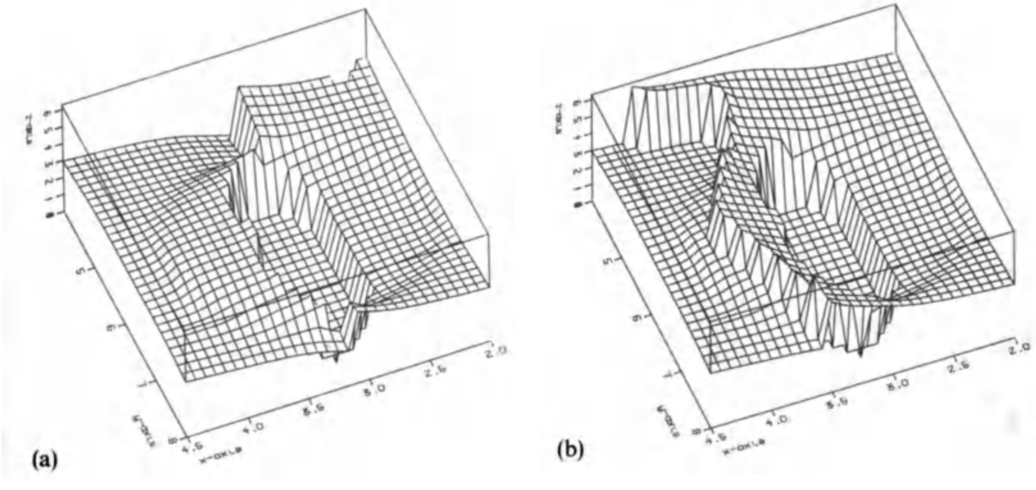


Figure 13 (a) and (b) A magnification of another part of the surface in Figure 10 (a) and (b).

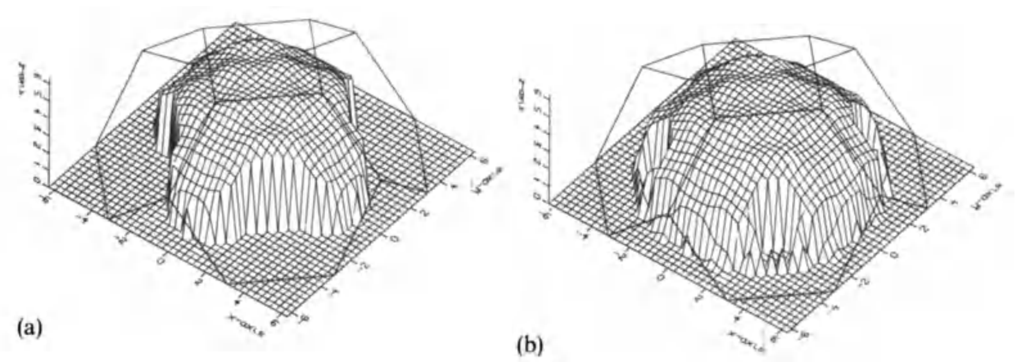


Figure 14 (a) and (b) The Fermi surface of a face centered cubic (FCC or cubic F) crystal with $E = -1$, $\alpha = -0.17$ inside the upper half of the Brillouin zone.

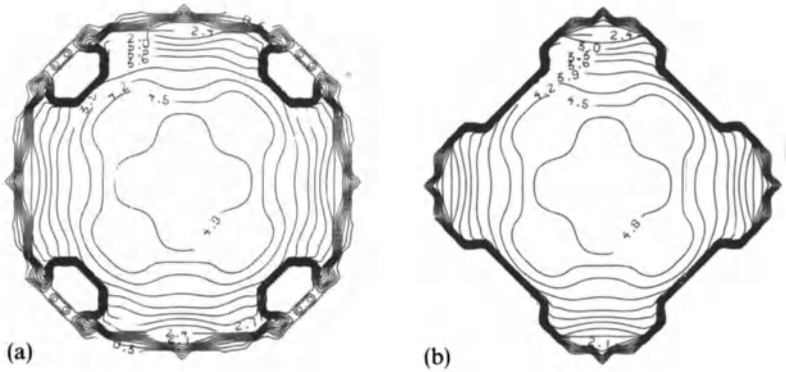


Figure 15 (a) and (b) A contour plot of Figure 14 (a) and (b).

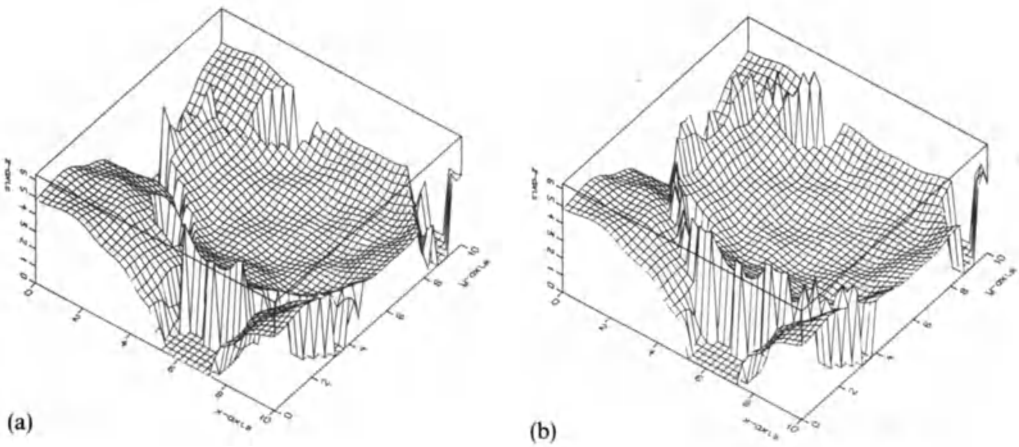
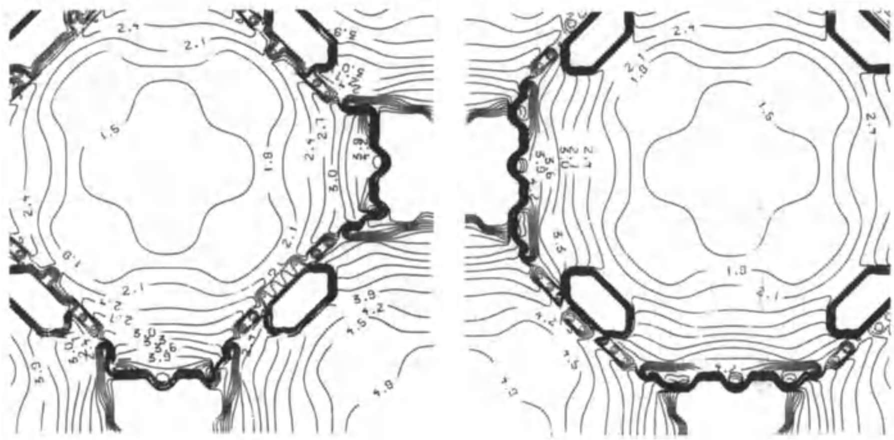
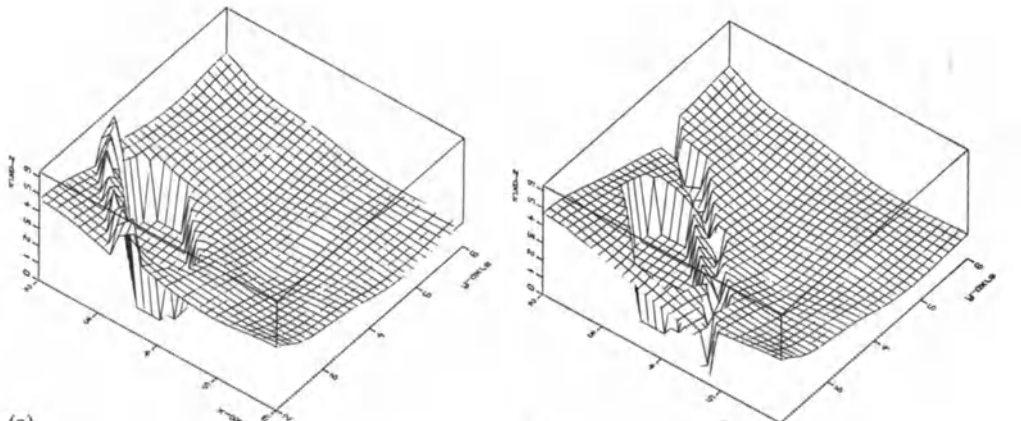


Figure 16 (a) and (b) The Fermi surface of Figure 14 extended periodically.



(a) (b)

Figure 17 (a) and (b) A contour plot of Figure 16 (a) and (b).



(a) (b)

Figure 18 (a) and (b) A magnification of a part of Figure 16 (a) and (b).

The next seven figures show how the Fermi surface inside the upper half of its Brillouin zone varies with E for an orthorhombic P crystal with axes $a = 3$, $b = 2$, $c = 1$ and with $\alpha = 0$.

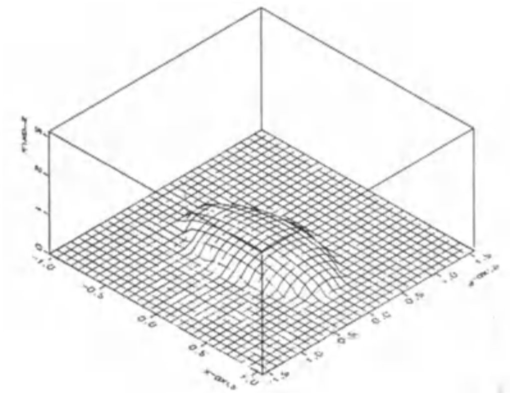


Figure 19 $E = -1.2$. The Fermi surface is homeomorphic to a sphere around each print of the orthogonal lattice.

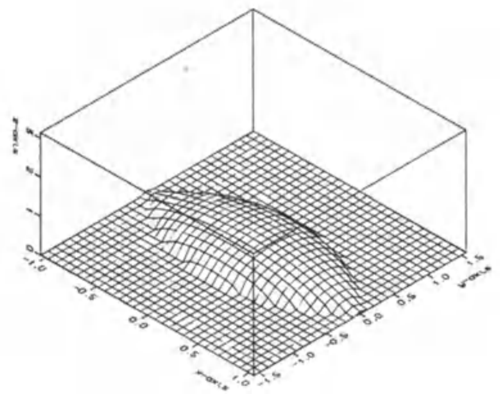


Figure 20 $E = -1.1$.

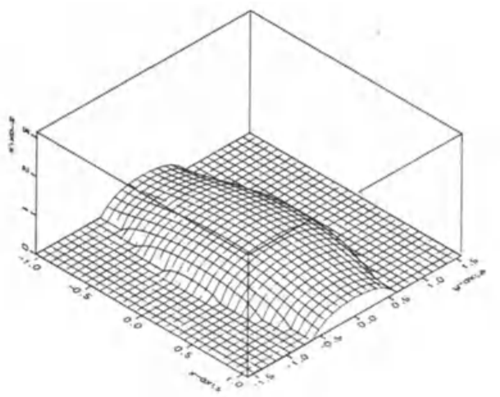


Figure 21 $E = -0.9$. The Fermi surface is now connected in the x-direction.

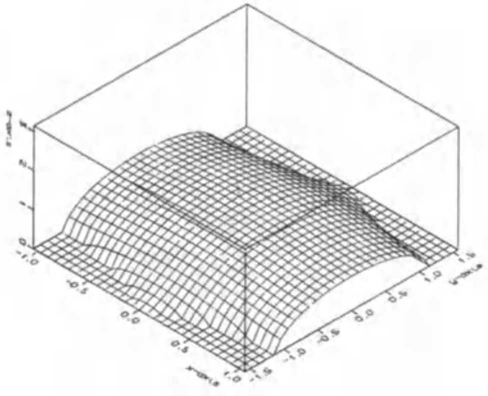


Figure 22 $E = -0.425$.

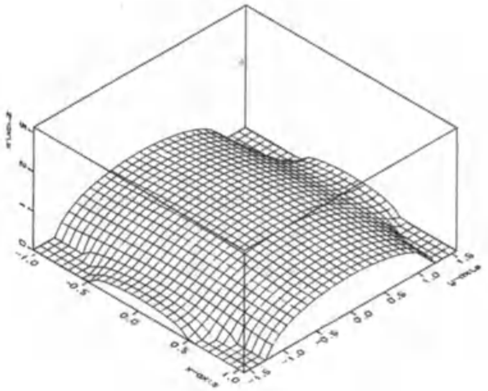


Figure 23 $E = -0.35$. The Fermi surface is connected in the x- and y-directions.

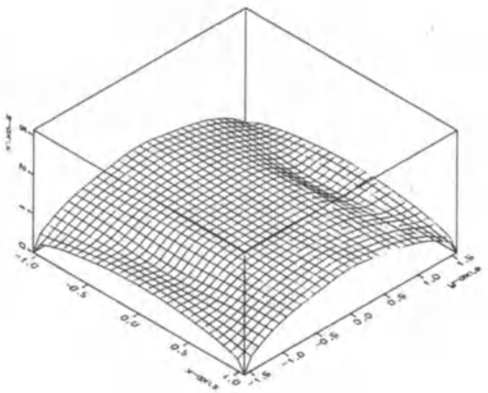


Figure 24 $E = -0.13$.

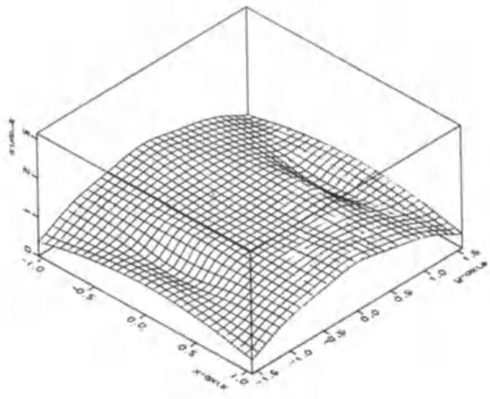


Figure 25 $E = -0.1$.

The next three figures show a similar series for a tetragonal P crystal with axes $a = b = 2$, $c = 1$ and with $\alpha = 0$.

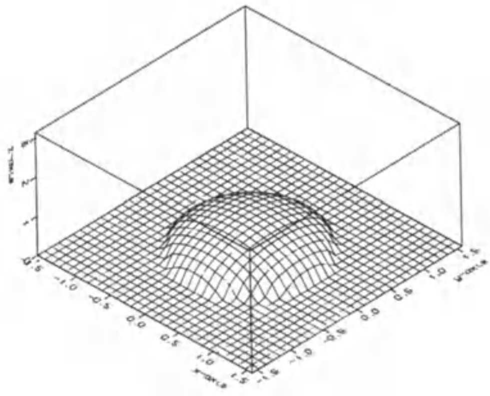


Figure 26 $E = -1.1$.

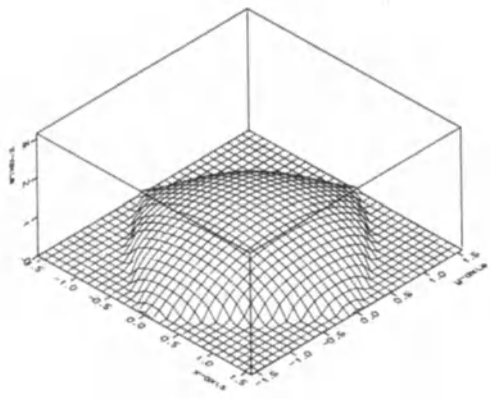


Figure 27 $E = -0.6$.

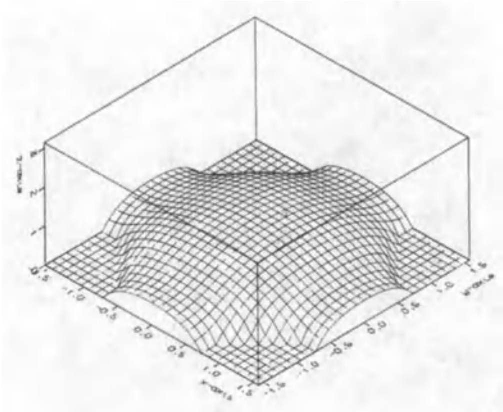


Figure 28 $E = -0.4$.

The next two figures show the Fermi surface inside the upper half of its Brillouin zone for a tetragonal P crystal with axes $a = b = 2$, $c = 3$ and with $\alpha = 0$ for two values of E.

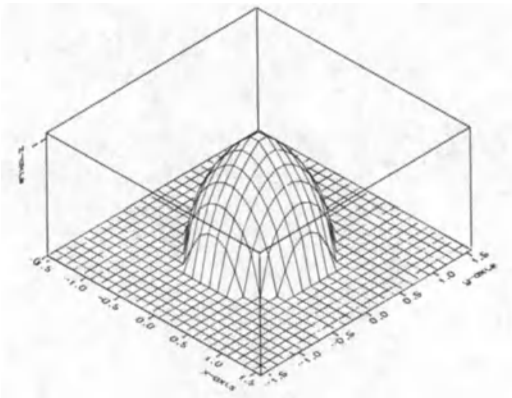


Figure 29 $E = -0.24$.

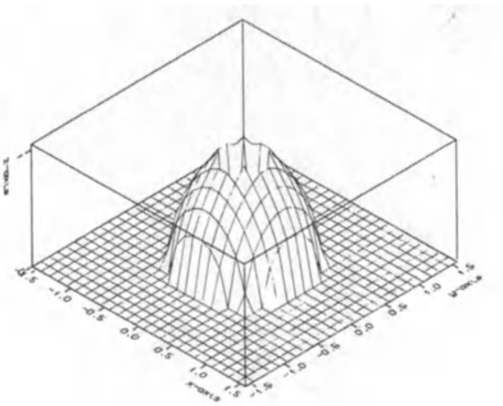


Figure 30 $E = -0.2$. The Fermi surface is now connected in the z-direction.

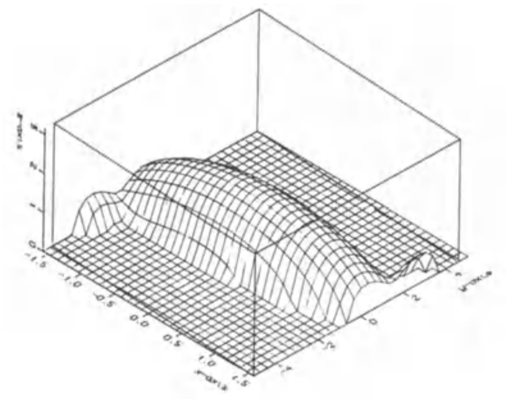


Figure 31 The surface for a monoclinic C crystal with axes $a = 2, b = 1.5, c = 1$ inside the upper half of its Brillouin zone. The angle between the axes $\vec{a}$ and $\vec{c}$ is 60°, $\alpha = 0$, and $E = -1$.

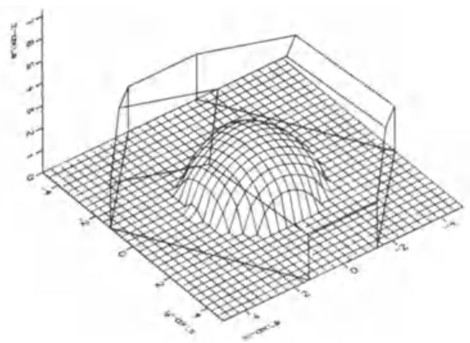


Fig. 32

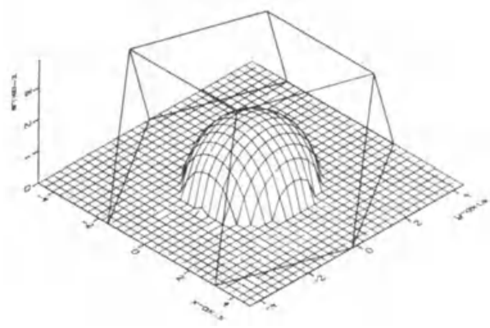


Fig. 33

Figures 32 and 33 The Fermi surfaces of a trigonal crystal with $\alpha = 0$ and $E = -1$ for two different angles, 30° and 70°, between the symmetry axis and each of the crystal axes.

III.1.9 Crystals with Defects and Impurities

Having studied in detail the spectral properties of a perfect, infinite crystal in three dimensions with point interactions, we now turn to the question of how various defects may change the spectrum in this model. As will turn out below, the point interaction Hamiltonian, in fact, allows one to make explicit computations of the consequences of certain defects.

Consider first the general situation where we have given

$$Y = \{y_j \in \mathbb{R}^3 \mid j \in J\}, \quad J \subseteq \mathbb{N}, \qquad \inf_{\substack{j,j' \in J \\ j \neq j'}} |y_j - y_{j'}| = d > 0, \qquad \alpha\colon Y \to \mathbb{R}, \tag{1.9.1}$$

with α bounded. We will study how the resolvent of the operator $-\Delta_{\alpha,Y}$ (given by (II.1.1.33) if $|Y| < \infty$ and by (1.1.6) if $|Y| = \infty$) is related to the resolvent of the operator $-\Delta_{\tilde{\alpha},\tilde{Y}}$ where $\tilde{\alpha}$ and $\tilde{Y}$ are certain modifications of α and Y, respectively. More precisely let

$$Z = \{z_1, \ldots, z_M\} \subset \mathbb{R}^3, \qquad M \in \mathbb{N}. \tag{1.9.2}$$

Then we distinguish the following three modifications:

(a) Assume that

$$\tilde{Y} = Y \cup Z, \qquad Y \cap Z = \varnothing, \quad Z \neq \varnothing,$$
$$\tilde{\alpha}|_Y = \alpha, \qquad \tilde{\alpha}_z = \beta_z \in \mathbb{R}, \quad z \in Z. \tag{1.9.3}$$

We then say that $-\Delta_{\tilde{\alpha},\tilde{Y}}$ represents the Hamiltonian with *interstitial impurities* located at $Z \subset \mathbb{R}^3$ relative to $-\Delta_{\alpha,Y}$, and write $-\Delta_{\alpha,Y,\beta,Z}$ for $-\Delta_{\tilde{\alpha},\tilde{Y}}$.

(b) Assume that

$$Y = \tilde{Y} \cup Z, \qquad \tilde{Y} \cap Z = \varnothing, \quad Z \neq \varnothing,$$
$$\alpha|_{\tilde{Y}} = \tilde{\alpha}, \qquad \alpha_z \in \mathbb{R}, \quad z \in Z. \tag{1.9.4}$$

We then say that $-\Delta_{\tilde{\alpha},\tilde{Y}}$ is the Hamiltonian with *defect impurities* or *vacancies* located at Z relative to $-\Delta_{\alpha,Y}$, and we write $-\Delta_{\alpha,Y,\{\infty\},Z}$ for $-\Delta_{\tilde{\alpha},\tilde{Y}}$.

(c) If

$$Y = \tilde{Y} = Z \cup \tilde{Z}, \qquad Z \cap \tilde{Z} = \varnothing, \quad Z, \tilde{Z} \neq \varnothing,$$
$$\tilde{\alpha}_y = \alpha_y \quad \text{iff} \quad y \in \tilde{Z}, \qquad \tilde{\alpha}_z = \beta_z \in \mathbb{R}, \quad z \in Z, \tag{1.9.5}$$

we say that $-\Delta_{\tilde{\alpha},\tilde{Y}}$ is the Hamiltonian representing *substitutional impurities* relative to $-\Delta_{\alpha,Y}$ and again we write $-\Delta_{\alpha,Y,\beta,Z}$ for $-\Delta_{\tilde{\alpha},\tilde{Y}}$.

For simplicity we will not consider a mixture of the above three cases. For the relation between the resolvents of $-\Delta_{\alpha,Y}$ and $-\Delta_{\alpha,Y,\beta,Z}$ we have the following

Theorem 1.9.1. *Let* $\tilde{Y} = \{\tilde{y}_j \in \mathbb{R}^3 | j \in \tilde{J}\}$, $Y = \{y_j \in \mathbb{R}^3 | j \in J\}$, $\tilde{J}$, $J \subseteq \mathbb{N}$, *satisfy*

$$\inf_{\substack{j,j' \in \tilde{J} \\ j \neq j'}} |\tilde{y}_j - \tilde{y}_{j'}| = d > 0, \qquad \inf_{\substack{j,j' \in J \\ j \neq j'}} |y_j - y_{j'}| = d > 0 \tag{1.9.6}$$

and assume that $\tilde{\alpha}$: $\tilde{Y} \to \mathbb{R}$ *and* α: $Y \to \mathbb{R}$ *are bounded. Moreover, let*

$$Z = \{z_1, \ldots, z_M\} \subset \mathbb{R}^3, \qquad M \in \mathbb{N}. \tag{1.9.7}$$

(a) *Suppose that*

$$\tilde{Y} = Y \cup Z, \qquad Y \cap Z = \varnothing, \qquad \tilde{\alpha}|_Y = \alpha, \qquad \tilde{\alpha}_z = \beta_z \in \mathbb{R}, \quad z \in Z, \tag{1.9.8}$$

and let

$$-\Delta_{\alpha,Y,\beta,Z} = -\Delta_{\tilde{\alpha},\tilde{Y}}. \tag{1.9.9}$$

Then

$$(-\Delta_{\alpha,Y,\beta,Z} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1} + \sum_{j,j'=1}^{M} [\Gamma_{\alpha,Y,\beta,Z}(k)]_{jj'}^{-1} (\overline{G_{k,\alpha,Y}(\cdot, z_{j'})}, \cdot) G_{k,\alpha,Y}(\cdot, z_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}) \cap \rho(-\Delta_{\alpha,Y,\beta,Z}), \quad \operatorname{Im} k > 0, \tag{1.9.10}$$

where

$$G_{k,\alpha,Y}(x, x') = (-\Delta_{\alpha,Y} - k^2)^{-1}(x, x') = \tilde{G}_k(x - x') + \sum_{y,y' \in Y} [\Gamma_{\alpha,Y}(k)]_{yy'}^{-1} \tilde{G}_k(x - y) \tilde{G}_k(x' - y'),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0, \tag{1.9.11}$$

and

$$\Gamma_{\alpha,Y,\beta,Z}(k) = \left[\left(\beta_{z_j} - \frac{ik}{4\pi}\right)\delta_{jj'} - G_{k,\alpha,Y}(z_j, z_{j'})\right]_{j,j'=1}^{M}. \tag{1.9.12}$$

(b) *Assume that*

$$Y = \tilde{Y} \cup Z, \qquad \tilde{Y} \cap Z = \varnothing, \qquad \alpha|_{\tilde{Y}} = \tilde{\alpha}, \qquad \alpha_z \in \mathbb{R}, \quad z \in Z, \tag{1.9.13}$$

and let

$$-\Delta_{\alpha,Y,\{\infty\},Z} = -\Delta_{\tilde{\alpha},\tilde{Y}}. \tag{1.9.14}$$

Then

$$(-\Delta_{\alpha,Y,\{\infty\},Z} - k^2)^{-1} = (-\Delta_{\alpha,Y} - k^2)^{-1} - \sum_{j,j'=1}^{M} [\Gamma_{\tilde{\alpha},\tilde{Y},\alpha,Z}(k)]_{jj'}^{-1} (\overline{G_{k,\tilde{\alpha},\tilde{Y}}(\cdot, z_{j'})}, \cdot) G_{k,\tilde{\alpha},\tilde{Y}}(\cdot, z_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}) \cap \rho(-\Delta_{\alpha,Y,\{\infty\},Z}), \quad \operatorname{Im} k > 0. \tag{1.9.15}$$

(c) *Suppose that*

$$Y = \tilde{Y} = Z \cup \tilde{Z}, \qquad Z \cap \tilde{Z} = \varnothing,$$

$$\tilde{\alpha}_y = \alpha_y \quad \text{iff} \quad y \in \tilde{Z}, \qquad \tilde{\alpha}_z = \beta_z \in \mathbb{R}, \quad z \in Z, \tag{1.9.16}$$

and let

$$-\Delta_{\alpha,Y,\beta,Z} = -\Delta_{\tilde{\alpha},\tilde{Y}}. \tag{1.9.17}$$

Then

$$\begin{aligned}(-\Delta_{\alpha,Y,\beta,Z} - k^2)^{-1} &= (-\Delta_{\alpha,Y} - k^2)^{-1} \\ &\quad + \sum_{j,j'=1}^{M} \{[\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1} D_{\alpha,\beta}[\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1}\}_{jj'} \cdot \\ &\quad \cdot (\overline{G_{k,\alpha,\tilde{Z}}(\cdot, z_{j'}')}, \cdot) G_{k,\alpha,\tilde{Z}}(\cdot, z_j), \\ &k^2 \in \rho(-\Delta_{\alpha,Y}) \cap \rho(-\Delta_{\alpha,Y,\beta,Z}), \quad \operatorname{Im} k > 0. \end{aligned} \tag{1.9.18}$$

with

$$D_{\alpha,\beta} = [D_{jj'}^{\alpha,\beta}]_{j,j'=1}^{M}, \qquad D_{jj'}^{\alpha,\beta} = (\alpha_{z_j} - \beta_{z_j})\delta_{jj'}, \qquad j, j' = 1, \ldots, M. \tag{1.9.19}$$

PROOF. (a) Write

$$\Gamma_{\tilde{\alpha},\tilde{Y}}(k) = \Gamma_{\oplus}(k) - \Gamma_c(k), \tag{1.9.20}$$

where

$$\Gamma_{\oplus}(k) = \begin{bmatrix} \Gamma_{\beta,Z}(k) & 0 \\ 0 & \Gamma_{\alpha,Y}(k) \end{bmatrix} \tag{1.9.21}$$

and $\Gamma_c(k)$ couples the points in Z to Y, i.e.,

$$\Gamma_c(k) = \begin{bmatrix} 0 & G_k(Z, Y) \\ G_k(Y, Z) & 0 \end{bmatrix} \tag{1.9.22}$$

with

$$\begin{aligned} G_k(Z, Y)&: l^2(Y) \to l^2(Z), \qquad G_k(Z, Y) = \{G_k(z - y)\}_{z \in Z, y \in Y}, \\ G_k(Y, Z)&: l^2(Z) \to l^2(Y), \qquad G_k(Y, Z) = \{G_k(y - z)\}_{y \in Y, z \in Z}. \end{aligned} \tag{1.9.23}$$

Then

$$[\Gamma_{\tilde{\alpha},\tilde{Y}}(k)]^{-1} = [\Gamma_{\oplus}(k)]^{-1} + [\Gamma_{\oplus}(k)]^{-1}\Gamma_c(k)\{1 - [\Gamma_{\oplus}(k)]^{-1}\Gamma_c(k)\}^{-1}[\Gamma_{\oplus}(k)]^{-1} \tag{1.9.24}$$

for $\operatorname{Im} k$ sufficiently large. The inverse $\{1 - [\Gamma_{\oplus}(k)]^{-1}\Gamma_c(k)\}^{-1}$ can be expressed explicitly in terms of $[\Gamma_{\alpha,Y,\beta,Z}(k)]^{-1}$, namely

$$\{1 - [\Gamma_{\oplus}(k)]^{-1}\Gamma_c(k)\}^{-1}$$
$$= \begin{bmatrix} \Gamma^{-1}\Gamma_{\beta,Z}(k) & \Gamma^{-1}G_k(Z, Y) \\ [\Gamma_{\alpha,Y}(k)]^{-1}G(Y, Z)\Gamma^{-1} & 1_Y + [\Gamma_{\alpha,Y}(k)]^{-1}G_k(Y, Z)\Gamma^{-1}G_k(Z, Y) \end{bmatrix}, \tag{1.9.25}$$

where for convenience we have abbreviated

$$\Gamma = \Gamma_{\alpha,Y,\beta,Z}(k) \tag{1.9.26}$$

and 1_Y denotes the identity matrix on $l^2(Y)$. A tedious but straightforward computation then gives (1.9.10).

(b) follows from (a) since an interchange of $-\Delta_{\tilde{\alpha},\tilde{Y}}$ and $-\Delta_{\alpha,Y}$ yields case (a).

(c) Observe first that

$$(-\Delta_{\alpha,Y,\beta,Z} - k^2)^{-1} - (-\Delta_{\alpha,Y} - k^2)^{-1}$$
$$= \sum_{j,j' \in J} \{[\Gamma_{\tilde{\alpha},\tilde{Y}}(k)]^{-1}_{jj'} - [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'}\}(\overline{G_k(\cdot - y_{j'})}, \cdot)G_k(\cdot - y_j), \quad (1.9.27)$$

and the problem now consists of reducing the right-hand side to a rank $M = |Z|$ operator. To this end, we write

$$\Gamma_{\tilde{\alpha},\tilde{Y}}(k) = \begin{bmatrix} \Gamma_{\tilde{\alpha},Z}(k) & -G(Z,\tilde{Z}) \\ -G(\tilde{Z},Z) & \Gamma_{\alpha,\tilde{Z}}(k) \end{bmatrix}, \quad \Gamma_{\alpha,Y}(k) = \begin{bmatrix} \Gamma_{\alpha,Z}(k) & -G(Z,\tilde{Z}) \\ -G(\tilde{Z},Z) & \Gamma_{\alpha,\tilde{Z}}(k) \end{bmatrix} \quad (1.9.28)$$

with inverses

$$[\Gamma_{\tilde{\alpha},\tilde{Y}}(k)]^{-1}$$
$$= \begin{bmatrix} [\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1} & [\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1}G(Z,\tilde{Z})[\Gamma_{\alpha,\tilde{Z}}(k)]^{-1} \\ [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)[\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1} & [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}+[\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)[\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1} \end{bmatrix},$$

$$[\Gamma_{\alpha,Y}(k)]^{-1}$$
$$= \begin{bmatrix} [\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1} & [\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1}G(Z,\tilde{Z})[\Gamma_{\alpha,\tilde{Z}}(k)]^{-1} \\ [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)[\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1} & [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1} + [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)[\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1} \end{bmatrix}. \quad (1.9.29)$$

Hence

$$[\Gamma_{\tilde{\alpha},\tilde{Y}}(k)]^{-1} - [\Gamma_{\alpha,Y}(k)]^{-1} = \begin{bmatrix} H & HG(Z,\tilde{Z})[\Gamma_{\alpha,\tilde{Z}}(k)]^{-1} \\ [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)H & [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}G(\tilde{Z},Z)HG(Z,\tilde{Z}) \end{bmatrix}, \quad (1.9.30)$$

where

$$H = [\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1} - [\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1} = [\Gamma_{\alpha,\tilde{Z},\beta,Z}(k)]^{-1}D_{\alpha,\beta}[\Gamma_{\alpha,\tilde{Z},\alpha,Z}(k)]^{-1} \quad (1.9.31)$$

with

$$D_{\alpha,\beta} = [D^{\alpha,\beta}_{jj'}]^{M}_{j,j'=1}, \qquad D^{\alpha,\beta}_{jj'} = (\alpha_{z_j} - \beta_{z_j})\delta_{jj'}, \qquad j,j' = 1,\ldots,M. \quad (1.9.32)$$

Recalling that

$$G_{k,\alpha,\tilde{Z}}(x,x') = \tilde{G}_k(x-x') + \sum_{y,y' \in \tilde{Z}} [\Gamma_{\alpha,\tilde{Z}}(k)]^{-1}_{yy'}G_k(x-y)G_k(x'-y'),$$
$$k^2 \in \rho(-\Delta_{\alpha,\tilde{Z}}), \quad \operatorname{Im} k > 0, \quad x,x' \in \mathbb{R}^3 - Z, \quad x \neq x', \quad (1.9.33)$$

a straightforward calculation, combining (1.9.27), (1.9.30), and (1.9.31), gives (1.9.18).

■

Remark. The theorem is still valid, with obvious modifications if $Z = \{z_j | j \in \mathbb{N}\}$ (i.e., if $M = \infty$) provided $|z - z'| \geq d > 0$, $z, z' \in Z$, $z \neq z'$.

Observe the strong resemblance between (1.9.10) and say (II.1.1.31). This suggests that (1.9.10) could be proved along the lines of the proof of Theorem

II.1.1.1 with $-\Delta$ replaced by $-\Delta_{\alpha,Y}$ [31]. Furthermore, we infer that adding another point interaction amounts to a change by a rank-one operator for the corresponding resolvents.

By using the above explicit formulas for the resolvents we can deduce the following general spectral properties.

Theorem 1.9.2. *Let* $\tilde{Y} = \{\tilde{y}_j \in \mathbb{R}^3 | j \in \tilde{J}\}$, $Y = \{y_j \in \mathbb{R}^3 | j \in J\}$, $J, \tilde{J} \subseteq \mathbb{N}$, *satisfy*

$$\inf_{\substack{j,j' \in \tilde{J} \\ j \neq j'}} |\tilde{y}_j - \tilde{y}_{j'}| = d > 0, \qquad \inf_{\substack{j,j' \in J \\ j \neq j'}} |y_j - y_{j'}| = d > 0 \tag{1.9.34}$$

and assume $\alpha\colon Y \to \mathbb{R}$, $\tilde{\alpha}\colon \tilde{Y} \to \mathbb{R}$ *to be bounded. Let*

$$Z = \{z_1, \ldots, z_M\} \subset \mathbb{R}^3, \qquad M \in \mathbb{N}, \tag{1.9.35}$$

and suppose one of the following three cases:

(a) $\tilde{Y} = Y \cup Z$, $Y \cap Z = \varnothing$, $\tilde{\alpha}|_Y = \alpha$, $\tilde{\alpha}_z = \beta_z \in \mathbb{R}$, $z \in Z$.
(b) $Y = \tilde{Y} \cup Z$, $\tilde{Y} \cap Z = \varnothing$, $\alpha|_{\tilde{Y}} = \tilde{\alpha}$, $\alpha_z \in \mathbb{R}$, $\beta_z = \infty$, $z \in Z$.
(c) $Y = \tilde{Y} = Z \cup \tilde{Z}$, $Z \cap \tilde{Z} = \varnothing$, $\tilde{\alpha}_y = \alpha_y$ iff $y \in \tilde{Z}$, $\tilde{\alpha}_z = \beta_z$, $z \in Z$.

Then

$$\sigma_{\text{ess}}(-\Delta_{\alpha,Y,\beta,Z}) = \sigma_{\text{ess}}(-\Delta_{\alpha,Y}) \tag{1.9.36}$$

and if $(a, b) \subset \rho(-\Delta_{\alpha,Y})$, $-\infty \leq a < b < \infty$, *then* $(a, b) \cap \sigma(-\Delta_{\alpha,Y,\beta,Z})$ *consists of at most* $M = |Z|$ *eigenvalues counting multiplicity.*

Proof. Weyl's theorem ([391], p. 112) proves (1.9.36). The statement about the multiplicity of eigenvalues follows from [494], p. 246. ∎

In short, Theorem 1.9.2 proves that defects of the kinds (a), (b), (c) do not change the essential spectrum, but may add eigenvalues in all gaps in the spectrum, the total number of which cannot exceed the number of defects. To obtain more precise information about these eigenvalues, one has to analyze the pole structure of the coefficients of the rank M operator. Assuming that one has only detailed spectral information on the "perfect" Hamiltonian $-\Delta_{\alpha,Y}$, this requires that the rank M operator is expressed exclusively in terms of $-\Delta_{\alpha,Y}$. By examining the formulas in Theorem 1.9.1, we see that these requirements make the formulas for case (b) and (c) less suitable.

Next we turn to more detailed statements concerning changes in the spectrum when $Y = \Lambda$, Λ being a Bravais lattice in the sense of (1.4.3). For the notation we refer to Sect. 1.4.

Corollary 1.9.3. *Let* $Z = \{z_1, \ldots, z_M\} \subset \mathbb{R}^3$, $M \in \mathbb{N}$, $\alpha \in \mathbb{R}$, *and* $\beta\colon Z \to \mathbb{R}$. *Assume that either* $Z \cap \Lambda = \varnothing$, *i.e., that* Z *is the location of the interstitial impurities* (*case* (a)), *or that* $Z \subset \Lambda$, *i.e.,* Z *is the location of the substitutional impurities* (*case* (c)). *Then* $\sigma(-\Delta_{\alpha,\Lambda,\beta,Z}) \cap (-\infty, E_0^{\alpha,\Lambda}(0))$ *contains at most* M *eigenvalues counting multiplicity.*

If $\alpha < \alpha_{0,\Lambda}$, then also $\sigma(-\Delta_{\alpha,\Lambda,\beta,z}) \cap (E_0^{\alpha,\Lambda}(\theta_0), 0)$ contains at most M eigenvalues counting multiplicity.

Although case (b), i.e., the case of vacancies, could easily have been included here, it is omitted since in this case we can prove stronger results, using other techniques (cf. Corollary 1.9.6). In the case of a single interstitial impurity our information is more detailed.

Theorem 1.9.4. *Let $z \in \mathbb{R}^3 - \Lambda$ be the location of the interstitial impurity and let $\alpha, \beta \in \mathbb{R}$. Define*

$$A^{\alpha,\Lambda}(k, z) = \frac{ik}{4\pi} + |\hat{\Lambda}|^{-1} \int_{\hat{\Lambda}} d^3\theta [\alpha - g_k(0, \theta)]^{-1} |g_k(z, \theta)|^2. \quad (1.9.37)$$

Then $-\Delta_{\alpha,\Lambda,\beta,z}$ has exactly one simple eigenvalue $E_{\beta,z}^{\alpha,\Lambda} \in (-\infty, E_0^{\theta,\Lambda}(0))$ iff

$$\beta > A^{\alpha,\Lambda}(k_0^{\alpha,\Lambda}(0), z), \qquad k_0^{\alpha,\Lambda}(0) = i\sqrt{-E_0^{\alpha,\Lambda}(0)}. \quad (1.9.38)$$

If $\alpha < \alpha_{0,\Lambda}$, then $-\Delta_{\alpha,\Lambda,\beta,z}$ has, in addition, one simple eigenvalue $E_{\beta,z}^{\alpha,\Lambda} \in (E_0^{\alpha,\Lambda}(\theta_0), 0)$ iff

$$A^{\alpha,\Lambda}(k_0^{\alpha,\Lambda}(\theta_0), z) > \beta > A^{\alpha,\Lambda}(0, z), \qquad k_0^{\alpha,\Lambda}(\theta_0) = i\sqrt{-E_0^{\alpha,\Lambda}(\theta_0)}. \quad (1.9.39)$$

If $E_{\beta,z}^{\alpha,\Lambda} = (k_{\beta,z}^{\alpha,\Lambda})^2$, $\mathrm{Im}\, k_{\beta,z}^{\alpha,\Lambda} > 0$, is an eigenvalue of $-\Delta_{\alpha,\Lambda,\beta,z}$ as above, then $k = k_{\beta,z}^{\alpha,\Lambda}$ solves

$$\beta = A^{\alpha,\Lambda}(k_{\beta,z}^{\alpha,\Lambda}, z) \quad (1.9.40)$$

and the corresponding eigenfunction ψ reads

$$\psi(x) = G_{k_{\beta,z}^{\alpha,\Lambda},\alpha,\Lambda}(x, z), \qquad x \in \mathbb{R}^3 - (\Lambda \cup \{z\}). \quad (1.9.41)$$

PROOF. From Theorem 1.9.1 we know that the equation which determines possible eigenvalues $E = k^2 < 0$, $\mathrm{Im}\, k > 0$, in the gaps of the spectrum of the perfect crystal reads

$$\beta = \frac{ik}{4\pi} + G_{k,\alpha,\Lambda}(z, z). \quad (1.9.42)$$

Furthermore, we have

$$\begin{aligned} G_{k,\alpha,\Lambda}(x, x') &= \tilde{G}_k(x - x') + (\overline{G_k(x - \cdot)}, [\Gamma_{\alpha,\Lambda}(k)]^{-1} G_k(x' - \cdot))_{l^2(\Lambda)} \\ &= \tilde{G}_k(x - x') + (g_k(x, \cdot), [\alpha - g_k(0, \cdot)]^{-1} g_k(x', \cdot))_{L^2(\hat{\Lambda}; |\hat{\Lambda}|^{-1} d^3\theta)} \end{aligned} \quad (1.9.43)$$

using the Fourier transform (cf. the proof of Theorem 1.4.3). Since $G_{k,\alpha,\Lambda}(z, z)$ is monotone increasing in κ, $\kappa = -ik > 0$, the result follows. ∎

We now turn to the detailed analysis of defects in ordered alloys. More precisely, we consider the operator $-\Delta_{\alpha,Y+\Lambda}$, as given in Theorem 1.4.3, where α satisfies (1.4.54)

$$Y = \{y_1, \ldots, y_N\} \subset \hat{\Gamma} \quad (1.9.44)$$

and "turn off" the point interactions at some points Z in order to introduce vacancies in the ordered alloy.

Theorem 1.9.5. *Consider the operator* $-\Delta_{\alpha, Y+\Lambda}$ *where* $\alpha \in \mathbb{R}^N$, Λ *is a Bravais lattice and* Y *satisfies* (1.9.44). *Let* B_j *denote the* jth *negative energy band*

$$B_j = \{E \in (-\infty, 0) | \exists \theta \in \hat{\Lambda}: \gamma_j^{\alpha, \Lambda, Y}(E, \theta) = 0\}, \qquad j = 1, \ldots, N, \quad (1.9.45)$$

where $\gamma_1^{\alpha, \Lambda, Y}(E, \theta) \le \cdots \le \gamma_N^{\alpha, \Lambda, Y}(E, \theta)$ *are the eigenvalues of the matrix* $\Gamma_{\alpha, \Lambda, Y}(k, \theta)$, $E = k^2$, $\operatorname{Im} k > 0$. *Define*

$$E_-^{\alpha, \Lambda, Y} = \inf[\sigma(-\Delta_{\alpha, Y+\Lambda})], \qquad E_+^{\alpha, \Lambda, Y} = \sup\{\sigma(-\Delta_{\alpha, Y+\Lambda}) \cap (-\infty, 0)\} \quad (1.9.46)$$

and assume that

$$B_j \neq \varnothing, \qquad j = 1, \ldots, N, \quad (1.9.47)$$

and

$$E_+^{\alpha, \Lambda, Y} < 0. \quad (1.9.48)$$

Then

$$\sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}}) \subseteq [E_-^{\alpha, \Lambda, Y}, E_+^{\alpha, \Lambda, Y}] \cup [0, \infty) \quad (1.9.49)$$

for any set $\tilde{Y}$ *such that*

$$\tilde{Y} \subseteq Y + \Lambda, \qquad \tilde{\alpha}|_{\tilde{Y}} = \alpha. \quad (1.9.50)$$

Furthermore, $-\Delta_{\tilde{\alpha}, \tilde{Y}}$ *has exactly* $M = |\tilde{Y}|$ *eigenvalues counting multiplicity provided* $M < \infty$.

Remark. Conditions (1.9.47) are satisfied if, e.g., $\sigma(-\Delta_{\alpha, Y+\Lambda})$ consists of exactly N negative bands.

Proof. Observe first that the matrix $\Gamma_{\alpha, \Lambda, Y}(E) \equiv \Gamma_{\alpha, Y+\Lambda}(k)$, $E = k^2$, $\operatorname{Im} k > 0$, is strictly positive definite for $E < E_-^{\alpha, \Lambda, Y}$ and strictly negative definite for $E \in (E_+^{\alpha, \Lambda, Y}, 0)$. This can be seen as follows. Assume that there is an $\tilde{E} < E_-^{\alpha, \Lambda, Y}$ (analogously, $\tilde{E} \in (E_+^{\alpha, \Lambda, Y}, 0)$) such that $\Gamma_{\alpha, Y, \Lambda}(\tilde{E})$ is negative. Applying

$$\Gamma(E) = \int_{\hat{\Lambda}}^{\oplus} d^3\theta \, \Gamma(E, \theta), \qquad \Gamma(E, \theta) \equiv \Gamma_{\alpha, \Lambda, Y}(k, \theta), \quad (1.9.51)$$

which was proved in Theorem 1.4.3, we infer that there is a $\tilde{\theta} \in \hat{\Lambda}$ such that $\Gamma(\tilde{E}, \tilde{\theta})$ has at least one negative eigenvalue $\gamma_{j_0}^{\alpha, \Lambda, Y}(\tilde{E}, \tilde{\theta})$. $\gamma_{j_0}^{\alpha, \Lambda, Y}(E, \tilde{\theta})$, being monotone decreasing in E, remains negative for $E \in (\tilde{E}, 0)$. Let $\tilde{\tilde{E}} \in B_{j_0}$ (implying $\tilde{E} < \tilde{\tilde{E}}$). Then there exists a $\tilde{\tilde{\theta}} \in \hat{\Lambda}$ such that $\gamma_{j_0}^{\alpha, \Lambda, Y}(\tilde{\tilde{E}}, \tilde{\tilde{\theta}}) = 0$, and hence $\gamma_{j_0}^{\alpha, \Lambda, Y}(E, \tilde{\tilde{\theta}}) > 0$ for all $E < \tilde{\tilde{E}}$. Using now the continuity in θ of $\gamma_{j_0}^{\alpha, \Lambda, Y}(\tilde{E}, \theta)$ we conclude that there exists a $\bar{\theta} \in \hat{\Lambda}$ such that $\gamma_{j_0}^{\alpha, \Lambda, Y}(\tilde{E}, \bar{\theta}) = 0$ which contradicts the definition of $E_-^{\alpha, \Lambda, Y}$. To prove (1.9.49) it suffices to prove that the matrix $\Gamma_{\tilde{\alpha}, \tilde{Y}}(k)$, $E = k^2$, $\operatorname{Im} k > 0$, is strictly positive definite for $k^2 < E_-^{\alpha, \Lambda, Y}$ and strictly negative definite for $k^2 \in (E_+^{\alpha, \Lambda, Y}, 0)$. From the min–max theorem ([391], Theorem XIII.1) we have

$$\inf[\sigma(\Gamma_{\tilde{\alpha}, \tilde{Y}}(k))] \ge \inf[\sigma(\Gamma(k^2))] > 0 \quad (1.9.52)$$

when $k^2 < E_-^{\alpha,\Lambda,Y}$, and

$$\sup[\sigma(\Gamma_{\tilde{\alpha},\tilde{Y}}(k))] \leq \sup[\sigma(\Gamma_{\alpha,Y}(k^2))] < 0 \tag{1.9.53}$$

when $k^2 \in (E_+^{\alpha,\Lambda,Y}, 0)$. The strict monotonicity in $E = k^2$ (for $E < 0$) of $\Gamma_{\tilde{\alpha},\tilde{Y}}(k)$ proves the statement about the multiplicity. ■

Corollary 1.9.6. *Let $\alpha \in \mathbb{R}$ and assume $Y \subseteq \Lambda$ to be an arbitrary subset of the lattice $\Lambda \subset \mathbb{R}^3$. Then*

$$\sigma(-\Delta_{\alpha,Y}) \subseteq [E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)] \cup [0, \infty). \tag{1.9.54}$$

If $\Lambda - Y$ is finite, i.e., if

$$|\Lambda - Y| < \infty, \tag{1.9.55}$$

then

$$\sigma(-\Delta_{\alpha,Y}) \cap (-\infty, 0) = [E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)] \tag{1.9.56}$$

provided $\alpha < \alpha_{0,\Lambda}$.

PROOF. Theorem 1.4.5 ensures that the conditions (1.9.47) and (1.9.48) are satisfied. From Theorem 1.9.1 we know that under assumption (1.9.55) $(-\Delta_{\alpha,\Lambda} - k^2)^{-1} - (-\Delta_{\alpha,Y} - k^2)^{-1}$ has rank $|\Lambda - Y| < \infty$, and hence the two operators have the same essential spectrum. ■

Before we study defects in binary ordered alloys, i.e., when $Y = \{y_1, y_2\}$, we will describe the spectrum of $-\Delta_{(\alpha_1,\alpha_2),\{y_1,y_2\}+\Lambda}$ in more detail.

Theorem 1.9.7. *Let $(\alpha_1, \alpha_2) \in \mathbb{R}^2$, $\alpha_1 < \alpha_2$, and let $\Lambda \subset \mathbb{R}^3$ be a Bravais lattice. If $y_1, y_2 \in \hat{\Gamma}$ and*

$$\sigma(-\Delta_{\alpha_1,\Lambda}) \cap \sigma(-\Delta_{\alpha_2,\Lambda}) \subseteq [0, \infty), \tag{1.9.57}$$

then

$$\sigma(-\Delta_{(\alpha_1,\alpha_2),\{y_1,y_2\}+\Lambda}) \cap (E_0^{\alpha_1,\Lambda}(\theta_0), E_0^{\alpha_2,\Lambda}(0)) = \varnothing. \tag{1.9.58}$$

PROOF. Observe first that

$$\sigma(-\Delta_{\alpha,\Lambda}) = \sigma(-\Delta_{\alpha,\{y\}+\Lambda}), \qquad y \in \mathbb{R}^3, \tag{1.9.59}$$

by translation invariance. Let $\theta \in \hat{\Lambda}$. By explicit computation

$$\gamma_1(k, \theta) \leq \alpha_1 - g_k(0, \theta) < \alpha_2 - g_k(0, \theta) \leq \gamma_2(k, \theta), \tag{1.9.60}$$

where $\gamma_1(k, \theta) < \gamma_2(k, \theta)$ are the eigenvalues of $\Gamma_{(\alpha_1,\alpha_2),\{y_1,y_2\}+\Lambda}(k, \theta)$. Furthermore, for $k^2 \in (E_0^{\alpha_1,\Lambda}(\theta_0), E_0^{\alpha_2,\Lambda}(0))$, we have

$$\alpha_1 - g_k(0, \theta) < 0 < \alpha_2 - g_k(0, \theta) \tag{1.9.61}$$

implying

$$\gamma_1(k, \theta) < 0 < \gamma_2(k, \theta) \tag{1.9.62}$$

and hence (1.9.58). ■

Turning now to defect impurities in ordered alloys we can state the following

Theorem 1.9.8. *Let $\alpha = (\alpha_1, \alpha_2) \in \mathbb{R}^2$, and let Λ be a Bravais lattice. Furthermore, let $Y = \{y_1, y_2\} \subset \hat{\Gamma}$ and assume that*

$$E_+^{\alpha, \Lambda, Y} < 0 \tag{1.9.63}$$

and

$$E_0^{\alpha_1, \Lambda}(\theta_0) < E_0^{\alpha_2, \Lambda}(0). \tag{1.9.64}$$

Let $\tilde{Y}$ be an arbitrary finite subset of $Y + \Lambda$, i.e.,

$$\tilde{Y} = \{y_1 + \lambda_{11}, \ldots, y_1 + \lambda_{N_1 1}\} \cup \{y_2 + \lambda_{12}, \ldots, y_2 + \lambda_{N_2 2}\} \subset Y + \Lambda \tag{1.9.65}$$

and $\tilde{\alpha} = \alpha|_{\tilde{Y}}$. Then

$$\begin{aligned} |\sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}}) \cap [E_-^{\alpha, \Lambda, Y}, E_0^{\alpha_1, \Lambda}(\theta_0)]| &= N_1, \\ |\sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}}) \cap [E_0^{\alpha_2, \Lambda}(0), E_+^{\alpha, \Lambda, Y}]| &= N_2, \end{aligned} \tag{1.9.66}$$

counting multiplicity.

PROOF. From Theorems 1.9.5 and 1.9.7 it follows that the negative part of $\sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}})$ consists of exactly $N_1 + N_2$ points within the two intervals $[E_-^{\alpha, \Lambda, Y}, E_+^{\alpha, \Lambda, Y}] - (E_0^{\alpha_1, \Lambda}(\theta_0), E_0^{\alpha_2, \Lambda}(0))$—so what remains to be proven is that they distribute in the stated way. This is shown using induction and Rayleigh's theorem. Assume that for given N_1 and N_2

$$\begin{aligned} \sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}}) \cap [E_-^{\alpha, \Lambda, Y}, E_0^{\alpha_1, \Lambda}(\theta_0)] &= \{E_1^{\tilde{Y}}, \ldots, E_{N_1}^{\tilde{Y}}\}, \\ \sigma(-\Delta_{\tilde{\alpha}, \tilde{Y}}) \cap [E_0^{\alpha_2, \Lambda}(0), E_+^{\alpha, \Lambda, Y}] &= \{E_{N_1+1}^{\tilde{Y}}, \ldots, E_N^{\tilde{Y}}\}, \end{aligned} \tag{1.9.67}$$

with $N = N_1 + N_2 = |Y|$ *and*

$$E_1^{\tilde{Y}} \leq \cdots \leq E_N^{\tilde{Y}}. \tag{1.9.68}$$

(In this and in the remaining part of the proof, all statements include possible degeneracies.) Let now

$$Y_1 = \tilde{Y} \cup \{y_1 + \lambda\}, \qquad y_1 + \lambda \in \tilde{Y}, \quad \lambda \in \Lambda. \tag{1.9.69}$$

Rayleigh's theorem ([391], Problem 11, p. 364) implies

$$E_1^{Y_1} \leq \cdots \leq E_N^{Y_1} \leq E_{N+1}^{Y_1}. \tag{1.9.70}$$

Suppose $E_{N_1+1}^{Y_1} > E_0^{\alpha_1, \Lambda}(\theta_0)$. Then there are $N_2 + 1$ eigenvalues of $-\Delta_{\alpha, Y_1}$ greater than $E_0^{\alpha_1, \Lambda}(\theta_0)$, which is impossible by the following argument. Consider $Y_2 = Y_1 - \{y_2 + \tilde{\lambda}\}$, $y_2 + \tilde{\lambda} \in Y_1$. Applying again Rayleigh's theorem we know that $-\Delta_{\alpha, Y_2}$ has at least $N_2 + 1$ eigenvalues greater than $E_0^{\alpha_1, \Lambda}(\theta_0)$. By repeating this argument another $N_2 - 1$ times we obtain the operator $-\Delta_{\alpha, \bar{Y}}$ with $\bar{Y} = \{y + \lambda, y_1 + \lambda_{11}, \ldots, y_1 + \lambda_{N_1 1}\}$ with at least one eigenvalue greater than $E_0^{\alpha_1, \Lambda}(\theta_0)$ which contradicts Corollary 1.9.6. Hence

$$\begin{aligned} |\sigma(-\Delta_{\alpha, Y_1}) \cap [E_-^{\alpha, \Lambda, Y}, E_0^{\alpha_1, \Lambda}(\theta_0)]| &= N_1 + 1, \\ |\sigma(-\Delta_{\alpha, Y_1}) \cap [E_0^{\alpha_2, \Lambda}(0), E_+^{\alpha, \Lambda, Y}]| &= N_2. \end{aligned} \tag{1.9.71}$$

Similarly, one proves the analogous result when one adds a point $y_2 + \lambda$ to the set Y_1. Finally, we observe in the case $N_1 = 1$ and $N_2 = 0$ that

$$\begin{aligned}\sigma(-\Delta_{\tilde{\alpha},\tilde{Y}}) &\subseteq [E_0^{\alpha_1,\Lambda}(0), E_0^{\alpha_2,\Lambda}(\theta_0)] \cup [0, \infty) \\ &\subseteq [E_-^{\alpha,\Lambda,Y}, E_+^{\alpha,\Lambda,Y}] \cup [0, \infty).\end{aligned} \tag{1.9.72}$$

using Theorem 1.9.5 and Corollary 1.9.6. The case $N_1 = 0$, $N_2 = 1$ follows analogously. ■

For binary ordered alloys we can improve Theorem 1.9.5.

Theorem 1.9.9. *Let $\alpha = (\alpha_1, \alpha_2) \in \mathbb{R}^2$, let Λ be a Bravais lattice, and let $Y = \{y_1, y_2\} \subset \hat{\Gamma}$. Assume that*

$$E_0^{\alpha_1,\Lambda}(\theta_0) < E_0^{\alpha_2,\Lambda}(0). \tag{1.9.73}$$

Then for any set $\tilde{Y}$ such that

$$\tilde{Y} \subseteq Y + \Lambda \tag{1.9.74}$$

we obtain

$$\sigma(-\Delta_{\tilde{\alpha},\tilde{Y}}) \subseteq [E_-^{\alpha,\Lambda,Y}, E_0^{\alpha_1,\Lambda}(\theta_0)] \cup [E^{\alpha_2,\Lambda}(0), E_+^{\alpha,\Lambda,Y}] \cup [0, \infty) \tag{1.9.75}$$

where $\tilde{\alpha} = \alpha|_{\tilde{Y}}$.

Proof. Consider the operator $-\Delta_{\tilde{\alpha},\tilde{Y}_n}$ where

$$\tilde{Y}_n = \tilde{Y} \cap B_n \tag{1.9.76}$$

with B_n being a ball of radius n with center at the origin. Following the proof of Theorem 1.1.1 we infer that

$$\operatorname*{s-lim}_{n\to\infty} (-\Delta_{\tilde{\alpha},\tilde{Y}_n} - k^2)^{-1} = (-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}. \tag{1.9.77}$$

Using Theorem 1.9.8 and the fact that the spectrum cannot expand under limits in the strong resolvent sense ([388], Theorem VIII.24) we conclude that (1.9.75) is valid. ■

One can also make similar statements for ternary ordered alloys, i.e., $|Y| = 3$.

Let $(\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$, $\{y_1, y_2, y_3\} \subset \hat{\Gamma}$, and assume that the spectrum of all the binary ordered alloys which one can construct consists of two nonoverlapping negative bands bounded away from zero, i.e.,

$$\begin{aligned}&\sigma(-\Delta_{\{\alpha_j,\alpha_{j'}\},\Lambda,\{y_j,y_{j'}\}}) \cap (-\infty, 0) \\ &\qquad = [E_{01}^{\Lambda}(j,j'), E_{11}^{\Lambda}(j,j')] \cup [E_{02}^{\Lambda}(j,j'), E_{12}^{\Lambda}(j,j')], \\ &E_{11}^{\Lambda}(j,j') < E_{02}^{\Lambda}(j,j') < E_{12}^{\Lambda}(j,j') < 0, \qquad j \neq j', \quad j,j' = 1, 2, 3.\end{aligned} \tag{1.9.78}$$

Then we can prove the following

Theorem 1.9.10. *Let $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$, $Y = \{y_1, y_2, y_3\} \subset \hat{\Gamma}$, and assume* (1.9.78). *Let*

$$\begin{aligned}E_{1l}^{\Lambda} &= \min\{E_{1l}^{\Lambda}(j,j') | j \neq j', j,j' = 1, 2, 3,\}, \\ E_{0l}^{\Lambda} &= \max\{E_{0l}^{\Lambda}(j,j') | j \neq j', j,j' = 1, 2, 3,\}, \qquad l = 1, 2,\end{aligned} \tag{1.9.79}$$

and assume

$$E_{12}^{\Lambda} < E_{02}^{\Lambda}, \qquad E_{11}^{\Lambda} < E_{01}^{\Lambda}. \tag{1.9.80}$$

Then

$$(E_{12}^{\Lambda}, E_{02}^{\Lambda}) \cap \sigma(-\Delta_{\alpha,\Lambda,Y}) = \varnothing, \qquad (E_{11}^{\Lambda}, E_{01}^{\Lambda}) \cap \sigma(-\Delta_{\alpha,\Lambda,Y}) = \varnothing. \tag{1.9.81}$$

Remark. See Figure 34 for a possible situation.

PROOF. Let $\theta \in \hat{\Lambda}$, $E = k^2 < 0$, $\operatorname{Im} k > 0$. Consider the six distinct 2×2 matrices

$$\Gamma_{jj'}(k, \theta) = \Gamma_{\{\alpha_j, \alpha_{j'}\}, \Lambda, \{y_j, y_{j'}\}}(k, \theta), \qquad j \neq j', \quad j, j' = 1, 2, 3, \tag{1.9.82}$$

and let

$$\gamma_1^{jj'}(k, \theta) \leq \gamma_2^{jj'}(k, \theta), \qquad j \neq j', \quad j, j' = 1, 2, 3, \tag{1.9.83}$$

denote their eigenvalues. From Rayleigh's theorem we infer

$$\gamma_1^{\alpha,\Lambda,Y}(k, \theta) \leq \gamma_1^{jj'}(k, \theta) \leq \gamma_2^{\alpha,\Lambda,Y}(k, \theta) \leq \gamma_2^{jj'}(k, \theta) \leq \gamma_3^{\alpha,\Lambda,Y}(k, \theta), \tag{1.9.84}$$

where (cf. (1.9.60))

$$\gamma_1^{\alpha,\Lambda,Y}(k, \theta) \leq \gamma_2^{\alpha,\Lambda}(k, \theta) \leq \gamma_3^{\alpha,\Lambda}(k, \theta) \tag{1.9.85}$$

denote the eigenvalues of $\Gamma_{\alpha,\Lambda,Y}(k, \theta)$. Now we can follow the arguments in the proof of Theorem 1.9.7. ■

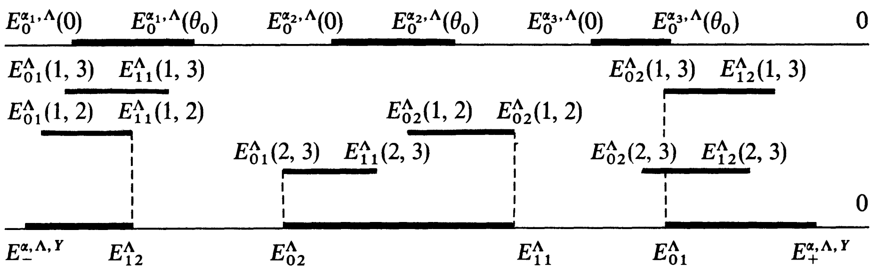


Figure 34

The analog of Theorem 1.9.8 now reads

Theorem 1.9.11. *Let* $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$, $\alpha_1 < \alpha_2 < \alpha_3$, *let* Λ *be a Bravais lattice, and let* $Y = \{y_1, y_2, y_3\} \subset \hat{\Gamma}$. *Furthermore, let* $\tilde{Y}$ *be an arbitrary finite subset of* $Y + \Lambda$, *i.e.,*

$$\tilde{Y} = \{y_1 + \lambda_{11}, \ldots, y_1 + \lambda_{N_1 1}\} \cup \{y_2 + \lambda_{12}, \ldots, y_2 + \lambda_{N_2 2}\}$$
$$\cup \{y_3 + \lambda_{13}, \ldots, y_3 + \lambda_{N_3 3}\} \subset Y + \Lambda \tag{1.9.86}$$

and assume that

$$E_0^{\alpha_1,\Lambda}(\theta_0) < E_{01}^{\Lambda}, \qquad E_0^{\alpha_3,\Lambda}(0) > E_{12}^{\Lambda}, \qquad E_+^{\alpha,\Lambda,Y} < 0. \tag{1.9.87}$$

Then

$$\begin{aligned}|\sigma(-\Delta_{\alpha,\Lambda,Y}) \cap [E_{-}^{\alpha,\Lambda,Y}, E_0^{\alpha_1,\Lambda}(\theta_0)]| &= N_1,\\ |\sigma(-\Delta_{\alpha,\Lambda,Y}) \cap [E_{01}^{\Lambda}, E_{12}^{\Lambda}]| &= N_2,\\ |\sigma(-\Delta_{\alpha,\Lambda,Y}) \cap [E_0^{\alpha_3,\Lambda}(0), E_{+}^{\alpha,\Lambda,Y}]| &= N_3,\end{aligned} \tag{1.9.88}$$

counting multiplicities.

PROOF. Similar to that of Theorem 1.9.8. ∎

Our last result concerning defects in ternary ordered alloys is the following analog of Theorem 1.9.9.

Theorem 1.9.12. *Let* $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3, \alpha_1 < \alpha_2 < \alpha_3,$ *let* Λ *be a Bravais lattice, and let* $Y = \{y_1, y_2, y_3\} \subset \hat{\Gamma}$. *Furthermore, let* $\tilde{Y}$ *be an arbitrary subset of* $Y + \Lambda$,

$$\tilde{Y} \subset Y + \Lambda \tag{1.9.89}$$

and assume (1.9.87). *Then*

$$\sigma(-\Delta_{\alpha,Y}) \subseteq [E_{-}^{\alpha,\Lambda,Y}, E_0^{\alpha_1,\Lambda}(0)] \cup [E_0^{\alpha_3,\Lambda}(\theta), E_{+}^{\alpha,\Lambda,Y}] \cup [0, \infty). \tag{1.9.90}$$

PROOF. Similar to that of Theorem 1.9.9. ∎

Notes

Section III.1.1

The presentation here is taken from Grossmann, Høegh-Krohn, and Mebkhout [227] which contains the first existence theorem in the general case of infinitely many centers.

Section III.1.2

The first approximation theorem in terms of local scaled short-range Hamiltonians in the infinite center case appeared in Albeverio and Høegh-Krohn [24]. They proved convergence in strong resolvent sense. This was later improved by [251], and we follow the latter approach although here for simplicity we only consider the case with a finite number of different potentials. The general case where all the potentials are allowed to be different is treated in [251] with additional assumptions on the potentials.

Section III.1.3

The one-electron model of an infinitely extended regular structure, e.g., a crystal, is one of the oldest models in quantum mechanics [290], [332], [391], [493]. The model, leading to a one-body Schrödinger operator with a periodic interaction, has been studied under the name of Floquet theory in mathematics and Bloch theory in physics. See also the notes to Sects 1.4 and 1.8.

Section III.1.4

The basic manipulations at the beginning of this section, due to [53], [54], are taken from Reed and Simon ([391], Sect. XIII.16), see also [85], [160], [443], [444]. The formula for the energy of the three-dimensional crystal with point interactions was first derived heuristically by Goldberger and Seitz in 1947 [216] (see also [479]), and was rediscovered by Grossmann, Høegh-Krohn, and Mebkhout [227]. A recent treatment appeared in [279]. Prior to [227] there had been some work on higher dimensional analogs of the Kronig–Penney model, which led to solvable models with certain nonseparable interactions [467]. The basic theorems, Theorems 1.4.4 and 1.4.5, are essentially taken from [227]. Theorem 1.4.1 and the consistency part of Theorem 1.4.3 are due to [249], while (1.4.47) is contained in [227]. Theorem 1.4.6 was proved in [243]. The approximation of $-\Delta_{\alpha,\Lambda}(\theta)$ in terms of local short-range Hamiltonians $H_{\varepsilon,\Lambda}(\theta)$ first appeared in [251], see also [178], and essentially we follow the former approach.

Section III.1.5

The formula for the energy bands was first derived heuristically by Demkov and Subramanian in 1970 [153], see also [88], [132], [151], [152], and later proved rigorously by Grossmann, Høegh-Krohn, and Mebkhout [227] (see also [281]). Here we essentially follow [227] while the approximation in terms of local scaled short-range Hamiltonians is taken from [251]. In [152] the problem is studied when the infinite straight polymer is replaced by a finite but long chain.

Section III.1.6

The model of an infinite monomolecular layer was first studied by Grossmann, Høegh-Krohn, and Mebkhout [227], from which its basic properties are taken. A recent treatment appeared in [280]. Theorem 1.6 appears to be new. The short-range expansion is taken from [251].

Section III.1.7

The results in this section were announced in [50], [52], but the detailed proof appears here for the first time. For general scattering theory off objects with different left and right space asymptotics, e.g., half-crystals, we refer to [136]. For Bragg scattering in the context of neutron scattering we refer to [141], [413].

Section III.1.8

The discussion in the first part of the section is essentially taken from [391], Ch. XIII. For the density of states for three-dimensional point interactions we refer to [215]. The illustrations of the Fermi surface are all taken from Høegh-Krohn, Holden, Johannesen, and Wentzel-Larsen [242]. For a comprehensive discussion of Fermi surfaces we refer to [126].

Section III.1.9

Theorem 1.9.1 is new, except for part (a) which is taken from Albeverio, Høegh-Krohn, and Mebkhout [31]. Their proof, however, is based on an analog of the proof of Theorem II.1.1.1, in which $-\Delta$ is replaced by $-\Delta_{\alpha,\Lambda}$, and which in turn is perturbed by a sum of point interactions located at Z.

Theorem 1.9.2, Corollary 1.9.3, and Theorem 1.9.4 appear to be new, while Theorems 1.9.5–1.9.12 are all taken from Høegh-Krohn, Holden, and Martinelli [243]. We also refer to [72], [391], and [481] for general results on impurity scattering.

CHAPTER III.2

Infinitely Many δ-Interactions in One Dimension

III.2.1 Basic Properties

In Sect. II.2.1 we studied δ-interactions centered at a finite set $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}$. The purpose of this section is to study the case $N \to \infty$ and hence treat the corresponding model with infinitely many centers.

Let $J \subset \mathbb{Z}$ be an infinite index set and let $Y = \{y_j \in \mathbb{R} \mid j \in J\}$ be a discrete subset of $\mathbb{R}$ such that for some $d > 0$

$$\inf_{\substack{j,j' \in J \\ j \neq j'}} |y_j - y_{j'}| = d > 0, \qquad y_j, y_{j'} \in Y, \quad j, j' \in J. \tag{2.1.1}$$

For notational convenience we assume that $j \in J$ implies $j + 1 \in J$ and $y_j < y_{j+1}$. We also define $I_j = [y_{j-1}, y_j], j - 1, j \in J$, and (with $j_{\inf} = \inf_{j \in J}(j)$) $I_{j_{\inf}} = (-\infty, y_{j_{\inf}}]$ in the case where $\inf Y = y_{j_{\inf}} > -\infty$ such that $\bigcup_{j \in J} I_j = \mathbb{R}$.

In analogy to Sect. II.2.1, we introduce the minimal operator $\dot{H}_Y$ in $L^2(\mathbb{R})$

$$\dot{H}_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}_Y) = \{g \in H^{2,2}(\mathbb{R}) | g(y_j) = 0, y_j \in Y, j \in J\} \tag{2.1.2}$$

and note that $\dot{H}_Y$ is closed and nonnegative. Its adjoint operator reads

$$\dot{H}_Y^* = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}_Y^*) = H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - Y). \tag{2.1.3}$$

The equation

$$\dot{H}_Y^* \psi(k) = k^2 \psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}_Y^*), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{2.1.4}$$

has the solutions

$$\psi_j(k, x) = e^{ik|x-y_j|}, \qquad \operatorname{Im} k > 0, \quad y_j \in Y, \quad j \in J, \tag{2.1.5}$$

which span the deficiency subspace of $\dot{H}_Y$. As a consequence $\dot{H}_Y$ has deficiency indices (∞, ∞). By the discussion in Appendix C a particular class of self-adjoint extensions of $\dot{H}_Y$ is of the type

$$-\Delta_{\alpha,Y} = -\frac{d^2}{dx^2},$$

$$\mathscr{D}(-\Delta_{\alpha,Y}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - Y) | g'(y_j+) - g'(y_j-) = \alpha_j g(y_j), j \in J\},$$

$$\alpha = \{\alpha_j\}_{j\in J}, \quad -\infty < \alpha_j \le \infty, \quad j \in J. \tag{2.1.6}$$

By definition $-\Delta_{\alpha,Y}$ describes δ-interactions of strength α_j centered at $y_j \in Y$, $j \in J$. The special case $\alpha_j = 0, j \in J$, represents the kinetic energy operator $-\Delta$ on $H^{2,2}(\mathbb{R})$, whereas $\alpha_{j_0} = \infty$ for some $j_0 \in J$ leads to a Dirichlet boundary condition at y_{j_0} (i.e., $g(y_{j_0}+) = g(y_{j_0}-) = 0$).

We start with an approximation of $-\Delta_{\alpha,Y}$ by means of finitely many δ-interactions.

Theorem 2.1.1. *Let $\alpha_j \in \mathbb{R}$, $j \in J$, and assume* (2.1.1). *Let $M, N \in \mathbb{N}$, $Y_{M,N} \subset Y$, $\alpha_{M,N} \subset \alpha$, where*

$$Y_{M,N} = \{y_j \in Y | -M \le j \le N\}, \qquad \alpha_{M,N} = \{\alpha_j\}_{j=-M}^{N}. \tag{2.1.7}$$

Then

$$(-\Delta_{\alpha_{M,N}, Y_{M,N}} - k^2)^{-1} \xrightarrow[M,N\to\infty]{s} (-\Delta_{\alpha,Y} - k^2)^{-1},$$

$$\operatorname{Im} k > 0, \quad k^2 \in \rho(-\Delta_{\alpha,Y}) \cap \rho_b, \tag{2.1.8}$$

where

$$\rho_b = \{z \in \mathbb{C} | z \in \rho(-\Delta_{\alpha_{M,N}, Y_{M,N}}) \text{ for } M, N \ge N_0(z), N_0(z) \in \mathbb{N} \text{ and }$$
$$\exists C\colon \|(-\Delta_{\alpha_{M,N}, Y_{M,N}} - z)^{-1}\| \le C \text{ for } M, N \ge N_0(z)\}. \tag{2.1.9}$$

PROOF. Let

$$\mathscr{D}_0 = \{f \in \mathscr{D}(-\Delta_{\alpha,Y}) | \operatorname{supp}(f) \text{compact}\}. \tag{2.1.10}$$

Then $\mathscr{D}_0$ is a core of $-\Delta_{\alpha,Y}$. For a proof of this fact let $f \in \mathscr{D}(-\Delta_{\alpha,Y})$ and truncate f by introducing

$$f_N = \phi_N f, \qquad N \in \mathbb{N}, \tag{2.1.11}$$

where

$$\phi_N \in C_0^\infty(\mathbb{R}), \qquad 0 \le \phi_N \le 1,$$

$$\phi_N(x) = \begin{cases} 1, & x \in \left[\dfrac{y_{-N+1} + y_{-N}}{2} + \dfrac{d}{4}, \dfrac{y_N + y_{N-1}}{2} - \dfrac{d}{4}\right], \\[2ex] 0, & x \le y_{-N} + \dfrac{d}{4} \text{ or } x \ge y_N - \dfrac{d}{4}, \end{cases} \tag{2.1.12}$$

$$\|\phi_N'\|_\infty + \|\phi_N''\|_\infty \le \text{const.}$$

Then $f_N \xrightarrow[N\to\infty]{s} f$ and

$$-\Delta_{\alpha,Y} f_N = \phi_N(-\Delta_{\alpha,Y} f) - 2\phi_N' f' - \phi_N'' f \xrightarrow[N\to\infty]{s} -\Delta_{\alpha,Y} f \tag{2.1.13}$$

by dominated convergence and the fact that $f' \in L^2(\mathbb{R})$. Next, let $g_0 \in \mathscr{D}_0$. Then $g_0 \in \mathscr{D}(-\Delta_{\alpha_{M,N}, Y_{M,N}})$ for $M, N \in \mathbb{N}$ sufficiently large and

$$-\Delta_{\alpha_{M,N}, Y_{M,N}} g_0 = -\Delta_{\alpha,Y} g_0 \tag{2.1.14}$$

completes the proof using Theorem VIII.1.5 of [283]. ■

By Theorem VIII.5.1 of [283] the above result implies

Theorem 2.1.2. *Let $\alpha_j \in \mathbb{R}, j \in J$, and assume (2.1.1). Let $\Omega \subset \mathbb{R}$ be any open set such that $\sigma(-\Delta_{\alpha,Y}) \subset \Omega$. Then the spectrum of $-\Delta_{\alpha_{M,N}, Y_{M,N}}$ is asymptotically concentrated on Ω, i.e.,*

$$P_{-\Delta_{\alpha_{M,N}, Y_{M,N}}}(\Omega) \xrightarrow[M,N\to\infty]{s} 1, \tag{2.1.15}$$

where $P_{-\Delta_{\alpha_{M,N}, Y_{M,N}}}(\cdot)$ denotes the spectral projection associated with $-\Delta_{\alpha_{M,N}, Y_{M,N}}$. Furthermore,

$$P_{-\Delta_{\alpha_{M,N}, Y_{M,N}}}((a, b)) \xrightarrow[M,N\to\infty]{s} P_{-\Delta_{\alpha,Y}}((a, b)), \qquad a, b \notin \sigma_p(-\Delta_{\alpha,Y}), \tag{2.1.16}$$

with $P_{-\Delta_{\alpha,Y}}(\cdot)$ the spectral projection of $-\Delta_{\alpha,Y}$.

Clearly, norm resolvent convergence cannot hold in (2.1.8) since, in general, $-\Delta_{\alpha,Y}$ has gaps in its essential spectrum (cf., e.g., Sect. 2.3) whereas $\sigma_{\text{ess}}(-\Delta_{\alpha_{M,N}, Y_{M,N}}) = [0, \infty)$ for all $M, N \in \mathbb{N}$.

Next we describe the resolvent of $-\Delta_{\alpha,Y}$.

Theorem 2.1.3. *Let $\alpha_j \in \mathbb{R} - \{0\}, j \in J$, and assume (2.1.1). Then*

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j' \in J} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} (\overline{G_k(\cdot - y_{j'})}, \cdot) G_k(\cdot - y_j),$$
$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \text{Im } k \geq 0, \tag{2.1.17}$$

where

$$\Gamma_{\alpha,Y}(k) = [-\alpha_j^{-1} \delta_{jj'} - G_k(y_j - y_{j'})]_{j,j' \in J}, \qquad \text{Im } k > 0, \tag{2.1.18}$$

is a closed operator in $l^2(Y)$ with

$$[\Gamma_{\alpha,Y}(k)]^{-1} \in \mathscr{B}(l^2(Y)), \quad k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \text{Im } k > 0 \text{ large enough.} \tag{2.1.19}$$

PROOF. We first prove that

$$\begin{aligned} f(k) &= \{(\overline{G_k(\cdot - y_j)}, f)\}_{j \in J} \in l^2(Y), \qquad \text{Im } k > 0, \\ g(k) &= \{(g, G_k(\cdot - y_j))\}_{j \in J} \in l^2(Y), \qquad \text{Im } k > 0, \end{aligned} \tag{2.1.20}$$

are analytic in $k^2 \in \mathbb{C} - [0, \infty)$. We estimate

$$\begin{aligned} |f(k)_j| &= \left| \sum_{n \in J} \int_{I_n} dx (i/2k) e^{ik|x - y_j|} f(x) \right| \\ &\leq (2|k|)^{-1} \sum_{n \in J_\infty} \left(\int_{I_n} dx \, e^{-2 \operatorname{Im} k |x - y_j|} \right)^{1/2} a_n, \end{aligned} \tag{2.1.21}$$

where

$$a_n = \left(\int_{I_n} dx\,|f(x)|^2\right)^{1/2}, \qquad n \in J, \quad a = \{a_n\}_{n\in J} \in l^2(J) \tag{2.1.22}$$

and I_n has been defined after (2.1.1). Introducing

$$M(k) = \{M(k)_{jn}\}_{j,n\in J}, \qquad M(k)_{jn} = \left(\int_{I_n} dx\, e^{-2\,\mathrm{Im}\,k|x-y_j|}\right)^{1/2}, \qquad \mathrm{Im}\,k > 0, \tag{2.1.23}$$

we want to prove that $M(k) \in \mathscr{B}(l^2(J))$. By explicit integration we get

$$\sum_{n\in J}\left(\int_{I_n} dx\, e^{-2\,\mathrm{Im}\,k|x-y_j|}\right)^{1/2} \le (2\,\mathrm{Im}\,k)^{-1/2} \sum_{n\in J} \begin{cases} e^{-\mathrm{Im}\,k|y_n-y_j|}, & n \le j, \\ e^{-\mathrm{Im}\,k|y_{n-1}-y_j|}, & n \ge j+1, \end{cases}$$
$$\le (2\,\mathrm{Im}\,k)^{-1/2} 2 \sum_{m\in\mathbb{Z}} e^{-\mathrm{Im}\,k|m|d}, \tag{2.1.24}$$

and hence

$$\|M(k)\|_H = \left(\sup_{j\in J}\sum_{n\in J}|M(k)_{jn}|\right)^{1/2}\left(\sup_{n\in J}\sum_{j\in J}|M(k)_{jn}|\right)^{1/2}$$
$$\le (2\,\mathrm{Im}\,k)^{-1/2} C < \infty, \tag{2.1.25}$$

where $\|\cdot\|_H$ denotes the Holmgren bound. Consequently, $M(k)$ is bounded in $l^2(J)$ and thus $f(k) \in l^2(Y)$. By the same estimates one proves analyticity of $f(k)$ in $k^2 \in \mathbb{C} - [0, \infty)$, $\mathrm{Im}\,k > 0$. Next let

$$g_k = [G_k(y_j - y_{j'})]_{j,j'\in J}, \qquad \mathrm{Im}\,k > 0. \tag{2.1.26}$$

Then $g_k \in \mathscr{B}(l^2(Y))$ since

$$\|g_k\|_H = \sup_{j\in J}\sum_{j'\in J}|G_k(y_j - y_{j'})| \le (2|k|)^{-1}\sup_{j\in J}\sum_{j'\in J} e^{-\mathrm{Im}\,k|y_j-y_{j'}|}$$
$$\le (2|k|)^{-1}\sup_{j\in J}\sum_{j'\in\mathbb{Z}} e^{-\mathrm{Im}\,k|j-j'|d} = (2|k|)^{-1}C' < \infty, \qquad \mathrm{Im}\,k > 0. \tag{2.1.27}$$

Thus $\|g_k\| = O(|\mathrm{Im}\,k|^{-1})$ as $\mathrm{Im}\,k \to \infty$ and $\Gamma_{\alpha,Y}(k)$ is closed in $l^2(Y)$ (self-adjoint for $k = i\kappa$, $\kappa > 0$). Decomposing g_k into its diagonal part $g_k^{\mathrm{D}} = (i/2k)1$ and off-diagonal part $g_k^{\mathrm{OD}} = g_k - g_k^{\mathrm{D}}$, the proof of (2.1.27) shows that

$$\|g_k^{\mathrm{OD}}\|_H \le (2|k|)^{-1}e^{-\mathrm{Im}\,kd}C'', \qquad \mathrm{Im}\,k > 0. \tag{2.1.28}$$

But the matrix

$$\{[-\alpha_j^{-1} - (i/2k)]\delta_{jj'}\}^{-1} = -\{[2\alpha_j k/(2k + i\alpha_j)]\delta_{jj'}\}_{j,j'\in J},$$
$$\mathrm{Im}\,k > 0, \quad k \neq -i\alpha_j/2, \quad j \in J, \tag{2.1.29}$$

is certainly bounded in $l^2(Y)$ implying $[\Gamma_{\alpha,Y}(k)]^{-1} \in \mathscr{B}(l^2(Y))$ for $\mathrm{Im}\,k > 0$ large enough, $k \neq -i\alpha_j/2$, $j \in J$. Moreover, g_k, $\mathrm{Im}\,k > 0$, is analytic in $k^2 \in \mathbb{C} - [0, \infty)$ and hence $[\Gamma_{\alpha,Y}(k)]^{-1}$ is analytic in $k^2 \in \mathbb{C} - [0, \infty)$ for $\mathrm{Im}\,k > 0$ large enough, $k \neq -i\alpha_j/2, j \in J$. Next we define in $l^2(Y)$

$$f_N(k) = \{f_N(k)_j\}_{j\in J}, \qquad g_N(k) = \{g_N(k)_j\}_{j\in J},$$
$$f_N(k)_j = \begin{cases} f(k)_j, & |j| \le N, \\ 0, & |j| \ge N+1, \end{cases} \qquad g_N(k)_j = \begin{cases} g(k)_j, & |j| \le N, \\ 0, & |j| \ge N+1, \end{cases}$$
$$j \in J, \quad N \in \mathbb{N}, \tag{2.1.30}$$

and

$$\Gamma_{\alpha,Y,N}(k) = [\Gamma_{\alpha,Y,N}(k)_{jj'}]_{j,j' \in J}$$

$$\Gamma_{\alpha,Y,N}(k)_{jj'} = \begin{cases} \Gamma_{\alpha,Y,N}(k)_{jj'}, & |j|, |j'| \le N, \\ 0, & |j| \ge N+1 \text{ or } |j'| \ge N+1; j, j' \in J, N \in \mathbb{N}. \end{cases} \tag{2.1.31}$$

Obviously, $f_N(k) \xrightarrow[N\to\infty]{s} f(k)$, $g_N(k) \xrightarrow[N\to\infty]{s} g(k)$, $\operatorname{Im} k > 0$, in $l^2(Y)$. Take $k = i\kappa$, $\kappa > 0$. Then $\Gamma_{\alpha,Y,N}(i\kappa)$, $N \in \mathbb{N}$, is bounded and self-adjoint with

$$\|\Gamma_{\alpha,Y,N}(i\kappa)\| \le \sup_{|j| \le N} |\alpha_j^{-1}| + (2\kappa)^{-1} C' \tag{2.1.32}$$

and $\Gamma_{\alpha,Y}(i\kappa)$ is self-adjoint. Let $a = \{a_j\}_{j\in J} \subset \mathscr{D}(\Gamma_{\alpha,Y}(i\kappa))$. Then $\lim_{N\to\infty} \|[\Gamma_{\alpha,Y,N}(i\kappa) - \Gamma_{\alpha,Y}(i\kappa)]a\| = 0$ since by splitting

$$\Gamma_{\alpha,Y,N}(i\kappa) \equiv \Gamma^{D}_{\alpha,Y,N}(i\kappa) + \Gamma^{OD}_{\alpha,Y,N}(i\kappa) \quad \text{and} \quad \Gamma_{\alpha,Y}(i\kappa) \equiv \Gamma^{D}_{\alpha,Y}(i\kappa) + \Gamma^{OD}_{\alpha,Y}(i\kappa)$$

into its diagonal and off-diagonal parts, respectively, the diagonal parts obviously fulfill $\lim_{N\to\infty} \|[\Gamma^{D}_{\alpha,Y,N}(i\kappa) - \Gamma^{D}_{\alpha,Y}(i\kappa)]a\| = 0$ and the off-diagonal terms are uniformly bounded and

$$\begin{aligned} \|[\Gamma^{OD}_{\alpha,Y,N}(i\kappa) - \Gamma^{OD}_{\alpha,Y}(i\kappa)]b\|^2 = &\sum_{\substack{|j| \ge N+1 \\ j\in J}} \left| \sum_{j'\in J} \Gamma^{OD}_{\alpha,Y}(i\kappa)_{jj'} b_{j'} \right|^2 \\ &+ \sum_{\substack{|j| \le N \\ j\in J}} \left| \sum_{\substack{|j'| \ge N+1 \\ j'\in J}} \Gamma^{OD}_{\alpha,Y}(i\kappa)_{jj'} b_{j'} \right|^2 \xrightarrow[N\to\infty]{} 0, \end{aligned}$$

$$b = \{b_j\}_{j\in J} \in l^2(Y), \tag{2.1.33}$$

since $\Gamma^{OD}_{\alpha,Y}(i\kappa)_{jj'} = -(1/2\kappa)e^{-\kappa|y_j - y_{j'}|} < 0, j \ne j', j, j' \in J$, and hence

$$\sum_{j\in J} \left[\sum_{j'\in J} |\Gamma^{OD}_{\alpha,Y}(i\kappa)_{jj'}| \, |b_{j'}| \right]^2 < \infty.$$

By Theorem VIII.1.5 in [283] we infer

$$[\Gamma_{\alpha,Y,N}(i\kappa)]^{-1} \xrightarrow[N\to\infty]{s} [\Gamma_{\alpha,Y}(i\kappa)]^{-1} \qquad \text{for } \kappa > 0 \text{ large enough}, \quad \kappa \ne -\alpha_j/2, \quad j \in J. \tag{2.1.34}$$

Finally, we use (cf. (II.2.1.6))

$$(f, (-\Delta_{\alpha_{N,N}, Y_{N,N}} - k^2)^{-1} g) = (f, G_k g) + (f_N(k), [\Gamma_{\alpha,Y,N}(k)]^{-1} g_N(k)),$$

$$\operatorname{Im} k > 0, \quad k^2 \in \rho(-\Delta_{\alpha_{N,N}, Y_{N,N}}), \tag{2.1.35}$$

where $(\cdot\,, \cdot)$ in the second term on the right-hand side of (2.1.35) denotes the scalar product in $l^2(Y)$. Taking $N \to \infty$ in (2.1.35), observing Theorem 2.1.1, (2.1.34), we obtain (2.1.17) in the weak sense for $k = i\kappa$, $\kappa > 0$, large enough, $\kappa \ne -\alpha_j/2, j \in J$. Using $\{G_k(\cdot - y_j)\}_{j\in J} \in l^2(Y)$, $\operatorname{Im} k > 0$, we infer (2.1.17) for $k = i\kappa$, $\kappa > 0$, large enough, $\kappa \ne -i\alpha_j/2, j \in J$. Analytic continuation with respect to $k^2 \in \rho(-\Delta_{\alpha,Y})$ then completes the proof. ∎

Additional properties of $-\Delta_{\alpha,Y}$ are described in

Theorem 2.1.4. *Let $\alpha_j \in \mathbb{R} - \{0\}, j \in J$, and assume* (2.1.1). *Then the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + \sum_{j,j'\in J} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} \phi_k(y_{j'}) G_k(x - y_j), \tag{2.1.36}$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ *and* $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k \geq 0$. *The decomposition* (2.1.36) *is unique and with* $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ *of this form we obtain*

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \tag{2.1.37}$$

Next let $\psi \in \mathscr{D}(-\Delta_{\alpha,Y})$ *and suppose that* $\psi = 0$ *in an open set* $U \subseteq \mathbb{R}$. *Then* $-\Delta_{\alpha,Y}\psi = 0$ *in* U.

PROOF. One can follow the corresponding proof of Theorem 1.1.2. ■

Finally, we describe an important one-to-one correspondence between $-\Delta_{\alpha,Y}$ in $L^2(\mathbb{R})$ and a certain discrete operator in $l^2(\mathbb{Z})$. Let $J = \mathbb{Z}$ and assume without loss of generality that $\pm\infty$ are accumulation points of Y implying $\mathbb{R} = \bigcup_{j\in\mathbb{Z}} I_j$ (otherwise, one could always take $\alpha_j = 0$ for all $j < j_{\text{inf}}$). Then the general solution of

$$(-\Delta_{\alpha,Y} - k^2)\psi(k,x) = 0, \qquad \operatorname{Im} k \geq 0, \quad x \in \mathring{I}_{j+1} = (y_j, y_{j+1}) \tag{2.1.38}$$

is given by

$$\begin{aligned}\psi(k,x) &= \psi(k,y_j)\cos[k(x-y_j)] + \psi'(k,y_j+)k^{-1}\sin[k(x-y_j)],\\ \psi'(k,x) &= -\psi(k,y_j)k\sin[k(x-y_j)] + \psi'(k,y_j+)\cos[k(x-y_j)],\\ &\qquad \operatorname{Im} k \geq 0, \quad x \in \mathring{I}_{j+1},\end{aligned} \tag{2.1.39}$$

with

$$\psi(k,y_j+) = \psi(k,y_j-), \qquad \psi'(k,y_j+) - \psi'(k,y_j-) = \alpha_j\psi(k,y_j), \qquad j \in \mathbb{Z}. \tag{2.1.40}$$

Introducing in $\mathbb{C}^2$

$$\Psi_j(k) = \begin{bmatrix} \psi(k,y_j) \\ \psi'(k,y_j-) \end{bmatrix},$$

$$T_j(k) = \begin{bmatrix} \cos[k(y_{j+1}-y_j)] + \alpha_j k^{-1}\sin[k(y_{j+1}-y_j)] & k^{-1}\sin[k(y_{j+1}-y_j)] \\ -k\sin[k(y_{j+1}-y_j)] + \alpha_j\cos[k(y_{j+1}-y_j)] & \cos[k(y_{j+1}-y_j)] \end{bmatrix},$$
$$\operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{2.1.41}$$

one infers from (2.1.40) that

$$T_j(k)\Psi_j(k) = \Psi_{j+1}(k), \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}. \tag{2.1.42}$$

Next we introduce in $\mathbb{C}^2$

$$W_j(k) = \begin{bmatrix} 1 & 0 \\ \cos[k(y_{j+1}-y_j)] & -k^{-1}\sin[k(y_{j+1}-y_j)] \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{2.1.43}$$

$$\Phi_j(k) = \begin{bmatrix} \psi(k,y_j) \\ \psi(k,y_{j-1}) \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{2.1.44}$$

and obtain

$$W_{j-1}(k)\Psi_j(k) = \Phi_j(k), \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{2.1.45}$$

and

$$[W_{j-1}(k)]^{-1} = -(k/\sin[k(y_j - y_{j-1})])\begin{bmatrix} -k^{-1}\sin[k(y_j - y_{j-1})] & 0 \\ -\cos[k(y_j - y_{j-1})] & 1 \end{bmatrix},$$
$$\operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}. \tag{2.1.46}$$

Defining

$$M_j(k)$$
$$= W_j(k)T_j(k)[W_{j-1}(k)]^{-1}$$
$$= \begin{bmatrix} \alpha_j k^{-1}\sin[k(y_{j+1} - y_j)] + \dfrac{\sin[k(y_{j+1} - y_{j-1})]}{\sin[k(y_j - y_{j-1})]} & -\dfrac{\sin[k(y_{j+1} - y_j)]}{\sin[k(y_j - y_{j-1})]} \\ 1 & 0 \end{bmatrix},$$
$$\operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \tag{2.1.47}$$

we get

$$M_j(k)\Phi_j(k) = \Phi_{j+1}(k), \quad \operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \tag{2.1.48}$$

or equivalently

$$\sin[k(y_j - y_{j-1})]\psi_{j+1}(k) + \sin[k(y_{j+1} - y_j)]\psi_{j-1}(k)$$
$$= \{\alpha_j k^{-1}\sin[k(y_{j+1} - y_j)]\sin[k(y_j - y_{j-1})] + \sin[k(y_{j+1} - y_{j-1})]\}\psi_j(k),$$
$$\operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \quad \psi_j(k) \equiv \psi(k, y_j),$$
$$\operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}. \tag{2.1.49}$$

Of course, (2.1.48) and (2.1.49) could have been derived directly (as we will do in Ch. 3) without introducing the second type of transfer matrices $T_j(k)$, $j \in \mathbb{Z}$.

We summarize this calculation in

Theorem 2.1.5. *Let* $\alpha_j \in \mathbb{R}$, $j \in J$, *and assume* (2.1.1). *Then any solution* $\psi(k, x)$, $k^2 \in \mathbb{R}$, $\operatorname{Im} k \geq 0$, $k \neq \pi m(y_j - y_{j-1})^{-1}, j, m \in \mathbb{Z}$, *of* (2.1.38) *(given by* (2.1.39) *and* (2.1.40)) *satisfies* (2.1.49). *Conversely, any solution of* (2.1.49) *defines via*

$$\psi(k, x) = \psi_j(k)\cos[k(x - y_j)]$$
$$+ \{\psi_{j+1}(k) - \psi_j(k)\cos[k(y_{j+1} - y_j)]\}\frac{\sin[k(x - y_j)]}{\sin[k(y_{j+1} - y_j)]},$$
$$x \in \mathring{I}_{j+1}, \quad k^2 \in \mathbb{R}, \quad \operatorname{Im} k \geq 0, \quad \kappa \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \tag{2.1.50}$$

a solution of (2.1.38) *(with* (2.1.39) *and* (2.1.40) *being valid). In addition,* $\psi(k) \in L^p(\mathbb{R})$ *implies* $\{\psi_j(k) = \psi(k, y_j)\}_{j \in \mathbb{Z}} \in l^p(\mathbb{Z})$ *for* $p = \infty$ *or* $p = 2$. *More-*

over, exponential growth (resp. decay) of $\psi(k, x)$ (i.e., $c_1 e^{\pm\delta|x|} \le |\psi(k, x)| \le c_2 e^{\pm\delta|x|}$) implies that of $\{\psi_j(k)\}_{j\in\mathbb{Z}}$ and at the same rate (i.e., $c_1' e^{\pm\delta|y_j|} \le |\psi_j(k)| \le c_2' e^{\pm\delta|y_j|}$). In the special case of a lattice structure of Y, i.e., $y_{j+1} - y_j = a > 0$, $j \in \mathbb{Z}$, the last two statements may be reversed, i.e., $\{\psi_j(k)\}_{j\in\mathbb{Z}} \in l^p(\mathbb{Z})$ implies $\psi(k) \in L^p(\mathbb{R})$ for $p = \infty$ or $p = 2$ and similarly for the exponential growth (resp. decay) rate.

PROOF. It remains to prove the last statements. Let $k^2 \in \mathbb{R}$, $\operatorname{Im} k \ge 0$, $k \ne \pi m(y_j - y_{j-1})^{-1}$, $j, m \in \mathbb{Z}$, and assume all solutions $\psi(k, x)$ and $\psi_j(k)$ to be real. If $\psi(k) \in L^p(\mathbb{R})$ and thus $\psi''(k) \in L^p(\mathbb{R})$ we infer $\psi'(k) \in L^p(\mathbb{R})$ ([283], p. 192) for all $1 \le p \le \infty$. Then $\{\psi_j(k) = \psi(k, y_j)\}_{j\in\mathbb{Z}} \in l^p(\mathbb{Z})$ follows from

$$\psi(k, y_j) = \psi(k, x)\cos[k(x - y_j)] - \psi'(k, x)k^{-1}\sin[k(x - y_j)], \quad x \in \mathring{I}_{j+1}, \tag{2.1.51}$$

for $p = \infty$ and from

$$[\psi(k, y_j)]^2 + k^{-2}[\psi'(k, y_j+)]^2 = [\psi(k, x)]^2 + k^{-2}[\psi'(k, x)]^2, \quad x \in \mathring{I}_{j+1}, \tag{2.1.52}$$

and (2.1.1) for $p = 2$. The assertions for the growth (resp. decay) rate are obtained as follows. From the Schrödinger equation we see that $\psi''(k, x)$ obeys the same inequalities as $\psi(k, x)$. The corresponding inequalities for $\psi'(k, x)$ now simply result after integration with respect to x. Conversely, assume $\{\psi_j(k)\}_{j\in\mathbb{Z}} \in l^p(\mathbb{Z})$ for $p = \infty$ or $p = 2$. The case $p = \infty$ directly results from (2.1.50) and the case $p = 2$ follows from (2.1.50) and

$$\begin{aligned}&[\psi(k, x)]^2 + k^{-2}[\psi'(k, x)]^2\\ &= [\psi_j(k)]^2 + \sin^{-2}[k(y_{j+1} - y_j)]\{\psi_{j+1}(k) - \psi_j(k)\cos[k(y_{j+1} - y_j)]\}^2, \quad x \in \mathring{I}_{j+1}.\end{aligned} \tag{2.1.53}$$

■

For later purposes we rewrite the basic formulas in the special case of a periodic lattice Y where $y_{j+1} - y_j = a > 0$, $y_j \in Y, j \in \mathbb{Z}$. Then the matrix $M_j(k)$ becomes

$$M_j(k) = \begin{bmatrix} \alpha_j k^{-1}\sin(ka) + 2\cos(ka) & -1 \\ 1 & 0 \end{bmatrix}, \quad \operatorname{Im} k \ge 0, \quad j \in \mathbb{Z}, \tag{2.1.54}$$

and (2.1.49) simply reads

$$\psi_{j+1}(k) + \psi_{j-1}(k) = \{\alpha_j k^{-1}\sin(ka) + 2\cos(ka)\}\psi_j(k),$$
$$\operatorname{Im} k \ge 0, \quad k \ne \pi m/a, \quad j, m \in \mathbb{Z}. \tag{2.1.55}$$

We emphasize that (2.1.38)–(2.1.40) lead directly to (2.1.55) implying the irrelevance of the exceptional points $k_m = \pi m/a$, $m \in \mathbb{Z}$, in this case. However, when starting from (2.1.55), to get back (2.1.38)–(2.1.40) one still encounters a $\frac{0}{0}$-term in (2.1.50) at the exceptional values $k_m = \pi m/a$, $m \in \mathbb{Z}$. It then depends on the sequence $\alpha = (\alpha_j)_{j\in\mathbb{Z}}$ whether $\psi(k, x)$ is well defined at such values k_m and hence whether there is a one-to-one correspondence between solutions of (2.1.38) (fulfilling (2.1.39) and (2.1.40)) and (2.1.55). In any case these exceptional points are irrelevant for determining the continuous spectrum of $-\Delta_{\alpha,Y}$.

III.2.2 Approximations by Means of Local Scaled Short-Range Interactions

The purpose of this section is to extend the approximation result of Sect. II.2.2 to the case of infinitely many centers. In addition to assumption (2.1.1) we introduce real-valued potentials $V_j \in L^1(\mathbb{R})$, $j \in J$, and $W \in L^1(\mathbb{R})$ such that almost everywhere

$$|V_j| \leq W, \qquad j \in J. \tag{2.2.1}$$

Define the quadratic forms in $L^2(\mathbb{R})$

$$q_{\varepsilon, y_j}(f, g) = \lambda_j(\varepsilon) \int_{\mathbb{R}} dx\, \varepsilon^{-2} V_j((x - y_j)/\varepsilon)\overline{f(x)}g(x), \qquad \mathscr{D}(q_{\varepsilon, y_j}) = H^{2,1}(\mathbb{R}),$$
$$0 < \varepsilon < \varepsilon_0, \quad j \in J, \tag{2.2.2}$$

and

$$q_{\alpha_j, y_j}(f, g) = \alpha_j \overline{f(y_j)} g(y_j), \qquad \mathscr{D}(q_{\alpha_j, y_j}) = H^{2,1}(\mathbb{R}), \qquad y_j \in Y, \quad j \in J, \tag{2.2.3}$$

with

$$\alpha_j \in \mathbb{R}, \qquad |\alpha_j| \leq C_0 < \infty, \qquad j \in J, \tag{2.2.4}$$

and $\lambda_j \in C^0((0, \varepsilon_0))$ real-valued for some $\varepsilon_0 > 0$ with

$$\lambda_j(\varepsilon) \underset{\varepsilon \downarrow 0}{=} \varepsilon\alpha_j + o(\varepsilon), \qquad j \in J. \tag{2.2.5}$$

By Lemma C.5

$$Q_{\alpha, Y}(f, g) = (f', g') + \sum_{j \in J} q_{\alpha_j, y_j}(f, g), \qquad \mathscr{D}(Q_{\alpha, Y}) = H^{2,1}(\mathbb{R}),$$
$$0 < \varepsilon < \varepsilon_0, \quad Y = \{y_j | j \in J\}, \tag{2.2.6}$$

and

$$Q_{\alpha, Y}(f, g) = (f', g') + \sum_{j \in J} q_{\alpha_j, y_j}(f, g), \qquad \mathscr{D}(Q_{\alpha, Y}) = H^{2,1}(\mathbb{R}),$$
$$\alpha = (\alpha_1, \alpha_2, \ldots), \tag{2.2.7}$$

are closed forms in $L^2(\mathbb{R})$ bounded from below. The unique self-adjoint and semibounded operator associated with $Q_{\varepsilon, Y}$ is denoted by $H_{\varepsilon, Y}$ and, as shown in Appendix C, the operator associated with $Q_{\alpha, Y}$ is precisely $-\Delta_{\alpha, Y}$ as defined in (2.1.6).

Our main result then reads

Theorem 2.2.1. *Assume* (2.1.1), V_j, $W \in L^1(\mathbb{R})$ *real-valued,* $|V_j| \leq W$, $0 < \varepsilon < \varepsilon_0$, $\lambda_j(\varepsilon) = \varepsilon\lambda_j'(0) + o(\varepsilon)$ *as* $\varepsilon \downarrow 0, j \in J$, *and let* $H_{\varepsilon, Y}$ *be defined as above. Then, as* $\varepsilon \downarrow 0$, $H_{\varepsilon, Y}$ *converges to* $-\Delta_{\alpha, Y}$ *in norm resolvent sense, i.e., if* $k^2 \in \rho(-\Delta_{\alpha, Y})$ *then* $k^2 \in \rho(H_{\varepsilon, Y})$ *for* $\varepsilon > 0$ *small enough and*

$$\operatorname*{n-lim}_{\varepsilon \downarrow 0} (H_{\varepsilon, Y} - k^2)^{-1} = (-\Delta_{\alpha, Y} - k^2)^{-1}, \qquad Y \subset \mathbb{R}, \tag{2.2.8}$$

where

$$\alpha_j = \lambda_j'(0) \int_{\mathbb{R}} dx\, V_j(x), \qquad j \in J. \tag{2.2.9}$$

PROOF. Let $f, g \in C_0^\infty(\mathbb{R})$ and

$$\eta_j \in C_0^\infty(\mathbb{R}), \quad 0 \le \eta_j \le 1, \quad \eta_j(x) = \begin{cases} 1, & |x - y_j| \le \delta, \\ 0, & |x - y_j| \ge 2\delta, \end{cases} \qquad \text{for some } 0 < \delta < d/4. \tag{2.2.10}$$

Then, for ε small enough, $j \in J$,

$$\begin{aligned}
&|q_{\varepsilon, y_j}(f, g) - q_{\alpha_j, y_j}(f, g)| \\
&\quad \le |\lambda_j'(0) + o(1)| \int_{y_j - \delta}^{y_j + \delta} dx\, \varepsilon^{-1} |V_j((x - y_j)/\varepsilon)|\, |\overline{f(x)} g(x) - \overline{f(y_j)} g(y_j)| \\
&\qquad + 2|\lambda_j'(0) + o(1)|\, \|f\|_\infty \|g\|_\infty \int_{(-\infty, y_j - \delta] \cup [y_j + \delta, \infty)} dx\, \varepsilon^{-1} |V_j((x - y_j)/\varepsilon)| \\
&\quad \le C \sup_{|x - y_j| \le \delta} |\overline{f(x)} g(x) - \overline{f(y_j)} g(y_j)| + C' \|f\|_\infty \|g\|_\infty \int_{(-\infty, -\delta/\varepsilon] \cup [\delta/\varepsilon, \infty)} dx\, W(x) \\
&\quad \le C \int_{y_j - 2\delta}^{y_j + 2\delta} dx\, \eta_j(x) [|f'(x)|\, |g(x)| + |f(x)|\, |g'(x)|] \\
&\qquad + C' \|f\|_\infty \|g\|_\infty \int_{(-\infty, -\delta/\varepsilon] \cup [\delta/\varepsilon, \infty)} dx\, W(x) \\
&\quad \le C \left(\int_{y_j - 2\delta}^{y_j + 2\delta} dx\, |\eta(x)|^2 \right)^{1/2} [\|f'\|\, \|g\|_\infty + \|f\|_\infty \|g'\|] \\
&\qquad + C' \|f\|_\infty \|g\|_\infty \int_{(-\infty, -\delta/\varepsilon] \cup [\delta/\varepsilon, \infty)} dx\, W(x) \\
&\quad \le C'' \left\{ \delta^{1/2} + \int_{(-\infty, -\delta/\varepsilon] \cup [\delta/\varepsilon, \infty)} dx\, W(x) \right\} \|f\|_{+1} \|g\|_{+1},
\end{aligned} \tag{2.2.11}$$

where

$$\|h\|_{+1}^2 \equiv \|h'\|^2 + \|h\|^2, \qquad h \in H^{2,1}(\mathbb{R}), \tag{2.2.12}$$

and ([389], p. 168)

$$\|h\|_\infty \le c \|h\|_{+1}, \qquad h \in H^{2,1}(\mathbb{R}), \tag{2.2.13}$$

have been used. Since $C_0^\infty(\mathbb{R})$ is a form core for $-\Delta$ on $H^{2,2}(\mathbb{R})$ and q_{ε, y_j}, q_{α_j, y_j} are infinitesimally bounded with respect to the kinetic energy form on $H^{2,1}(\mathbb{R})$, the estimate (2.2.11) extends to all $f, g \in H^{2,1}(\mathbb{R})$. Next, let $\phi_l, \psi_l \in H^{2,1}(\mathbb{R})$ and

$$\operatorname{supp}(\phi_l), \operatorname{supp}(\psi_l) \subset \left[dl - \frac{3d}{2}, dl + \frac{3d}{2} \right], \qquad l \in \mathbb{Z}.$$

Choose a dl_j, $l_j \in \mathbb{Z}$, which is closest to $y_j \in Y$. Then for $l = l_j, l_j \pm 1, l_j \pm 2$, the above method shows that for any $v > 0$ there exists an $0 < \varepsilon_1 < \varepsilon_0$ such that for all

$0 < \varepsilon \leq \varepsilon_1, j \in J,$

$$|q_{\varepsilon, y_j}(\phi_l, \psi_l) - q_{\alpha_j, y_j}(\phi_l, \psi_l)| \leq \nu \|\phi_l\|_{+1} \|\psi_l\|_{+1}, \qquad l = l_j, \quad l_j \pm 1, \quad l_j \pm 2. \quad (2.2.14)$$

For $l \in \mathbb{Z} - \{l_j, l_j \pm 1, l_j \pm 2\}$ we get from $\phi_l(y_j) = \psi_l(y_j) = 0, j \in J$,

$$\begin{aligned} |q_{\varepsilon, y_j}(\phi_l, \psi_l) - q_{\alpha_j, y_j}(\phi_l, \psi_l)| &= |q_{\varepsilon, y_j}(\phi_l, \psi_l)| \\ &\leq |\lambda_j'(0) + o(1)| \, \|\phi_l\|_\infty \|\psi_l\|_\infty \int_{(dl-(3d/2)-y_j)/\varepsilon}^{(dl+(3d/2)-y_j)/\varepsilon} dx \, W(x) \\ &\leq \tilde{c} \int_{(dl-(3d/2)-y_j)/\varepsilon}^{(dl+(3d/2)-y_j)/\varepsilon} dx \, W(x) \|\phi_l\|_{+1} \|\psi_l\|_{+1}, \\ &\qquad l \in \mathbb{Z} - \{l_j, l_j \pm 1, l_j \pm 2\}. \quad (2.2.15) \end{aligned}$$

From (2.2.14) and

$$\sum_{l \in \mathbb{Z} - \{l_j, l_j \pm 1, l_j \pm 2\}} \int_{(dl-(3d/2)-y_j)/\varepsilon}^{(dl+(3d/2)-y_j)/\varepsilon} dx \, W(x) \leq 3 \int_{-\infty}^{-1/2\varepsilon} dx \, W(x) + 3 \int_{1/2\varepsilon}^{\infty} dx \, W(x) \quad (2.2.16)$$

we actually infer that for any $\nu > 0$ there exists an $0 < \varepsilon_1 < \varepsilon_0$ such that for $0 < \varepsilon \leq \varepsilon_1, j \in J$,

$$|q_{\varepsilon, y_j}(\phi, \psi) - q_{\alpha_j, y_j}(\phi, \psi)| \leq a_l \|\phi\|_{+1} \|\psi\|_{+1}, \qquad j \in J, \quad (2.2.17)$$

for all $\phi, \psi \in H^{2,1}(\mathbb{R})$, $\operatorname{supp}(\phi)$, $\operatorname{supp}(\psi) \subset [dl - (3d/2), dl + (3d/2)]$ with

$$\sum_{l \in \mathbb{Z}} a_l < \nu. \quad (2.2.18)$$

Thus Lemma C.5 applies and yields for all $\nu > 0$

$$|Q_{\varepsilon, Y}(f, f) - Q_{\alpha, Y}(f, f)| \leq \nu \|f\|_{+1}^2, \qquad f \in H^{2,1}(\mathbb{R}), \quad (2.2.19)$$

implying

$$|Q_{\varepsilon, Y}(f, g) - Q_{\alpha, Y}(f, g)| \leq \nu \|f\|_{+1} \|g\|_{+1}, \qquad f, g \in H^{2,1}(\mathbb{R}). \quad (2.2.20)$$

But (2.2.20) implies norm resolvent convergence of $H_{\varepsilon, Y}$ to $-\Delta_{\alpha, Y}$ by Theorem VIII.25c of [388]. ■

We observe again that if $\lambda_{j_0}'(0) \int_{\mathbb{R}} dx \, V_{j_0}(x) = 0$ for some $j_0 \in J$, the δ-interaction at y_{j_0} disappears in $-\Delta_{\alpha, Y}$. In particular, $H_{\varepsilon, Y}$ converges to $-\Delta$ as $\varepsilon \downarrow 0$ if and only if $\lambda_j'(0) \int_{\mathbb{R}} dx \, V_j(x) = 0$ for all $j \in J$.

Obviously, our proof of Theorem 2.2.1 represents an alternative to the corresponding proofs of Theorems I.3.2.3 and II.2.2.2.

III.2.3 Periodic δ-Interactions

In this section we treat the case of periodic δ-interactions on the real line. We start with the simplest case of the Kronig–Penney model and subsequently discuss generalizations of it.

In the Kronig–Penney model the Bravais lattice Λ simply reads

$$\Lambda = \{na \mid n \in \mathbb{Z}\}, \qquad a > 0, \quad (2.3.1)$$

such that the Wigner–Seitz cell $\hat{\Gamma}$ is given by

$$\hat{\Gamma} = [-a/2, a/2). \tag{2.3.2}$$

The dual lattice Γ is then defined by

$$\Gamma = \{nb | n \in \mathbb{Z}\}, \qquad b = 2\pi/a, \tag{2.3.3}$$

and the Brillouin zone $\hat{\Lambda}$ equals

$$\hat{\Lambda} = [-b/2, b/2). \tag{2.3.4}$$

Then the Hilbert space $L^2(\mathbb{R})$ can be decomposed as

$$L^2(\mathbb{R}) = \mathscr{U}^{-1} L^2(\hat{\Lambda}; l^2(\Gamma)) \equiv \mathscr{U}^{-1} \int_{[-b/2, b/2)}^{\oplus} d\theta \, l^2(\Gamma), \tag{2.3.5}$$

where

$$\mathscr{U}: L^2(\mathbb{R}) \to L^2(\hat{\Lambda}; l^2(\Gamma)),$$
$$(\mathscr{U}f)(\theta, n) = \hat{f}(\theta + nb), \quad \theta \in [-b/2, b/2), \quad n \in \mathbb{Z}, \quad f \in L^2(\mathbb{R}), \tag{2.3.6}$$

or as

$$\begin{aligned} L^2(\mathbb{R}) &= \tilde{\mathscr{U}}^{-1} L^2(\hat{\Lambda}, b^{-1}\, d\theta; L^2([-a/2, a/2))) \\ &\equiv \tilde{\mathscr{U}}^{-1} \int_{[-b/2, b/2)}^{\oplus} \frac{d\theta}{b} L^2([-a/2, a/2)), \end{aligned} \tag{2.3.7}$$

where

$$\tilde{\mathscr{U}}: \mathscr{S}(\mathbb{R}) \to L^2(\hat{\Lambda}, b^{-1}\, d\theta; L^2([-a/2, a/2))),$$
$$(\tilde{\mathscr{U}}f)(\theta, v) = \sum_{n=-\infty}^{\infty} e^{in\theta a} f(v + na),$$
$$v \in [-a/2, a/2), \quad \theta \in [-b/2, b/2), \quad f \in \mathscr{S}(\mathbb{R}),$$
$$\tilde{\mathscr{U}}^{-1}: L^2(\hat{\Lambda}, b^{-1}\, d\theta; L^2([-a/2, a/2))) \to L^2(\mathbb{R}), \tag{2.3.8}$$
$$(\tilde{\mathscr{U}}^{-1} g)(v + na) = b^{-1} \int_{-b/2}^{b/2} d\theta \, e^{-in\theta a} g(\theta, v),$$
$$g \in L^2(\hat{\Lambda}, b^{-1}\, d\theta; L^2([-a/2, a/2))), \quad v \in [-a/2, a/2), \quad n \in \mathbb{Z},$$

where the closure of $\tilde{\mathscr{U}}$ is denoted by the same symbol.

Next we unitarily implement translations $x \to x + a$ in $L^2(\mathbb{R})$, i.e., we introduce the operator

$$(T_a f)(x) = f(x + a), \qquad f \in L^2(\mathbb{R}), \tag{2.3.9}$$

implying

$$T_a = \exp\left[ia\left(i^{-1}\frac{d}{dx}\right)\right], \qquad \mathscr{D}\left(i^{-1}\frac{d}{dx}\right) = H^{2,1}(\mathbb{R}). \tag{2.3.10}$$

Obviously, T_a is diagonal with respect to the decomposition (2.3.7), i.e.,

$$\tilde{\mathscr{U}} T_a \tilde{\mathscr{U}}^{-1} = \int_{[-b/2, b/2)}^{\oplus} \frac{d\theta}{b} e^{-i\theta a}. \tag{2.3.11}$$

(Note that θ is the so-called quasi momentum or Bloch's vector.) Now we are in a position to study the Kronig–Penney Hamiltonian $-\Delta_{\alpha,\Lambda}$ in $L^2(\mathbb{R})$ which according to (2.1.6) is defined as

$$-\Delta_{\alpha,\Lambda} = -\frac{d^2}{dx^2},$$
$$\mathscr{D}(-\Delta_{\alpha,\Lambda}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - \Lambda) | g'(na+) - g'(na-) = \alpha g(na),\ n \in \mathbb{Z}\},$$
$$-\infty < \alpha \leq \infty. \tag{2.3.12}$$

In addition, we introduce the family of self-adjoint operators in $L^2((-a/2, a/2))$

$$-\Delta_{\alpha,\Lambda}(\theta) = -\frac{d^2}{dv^2},$$
$$\mathscr{D}(-\Delta_{\alpha,\Lambda}(\theta)) = \{g(\theta) \in H^{2,1}((-a/2, a/2)) \cap H^{2,2}((-a/2, a/2) - \{0\})|\ g(\theta, -a/2+) = e^{i\theta a} g(\theta, a/2-),$$
$$g'(\theta, -a/2+) = e^{i\theta a} g'(\theta, a/2-),\ g'(\theta, 0+) - g'(\theta, 0-) = \alpha g(\theta, 0)\},$$
$$-\infty < \alpha \leq \infty, \quad \theta \in [-b/2, b/2), \tag{2.3.13}$$

(self-adjointness of $-\Delta_{\alpha,\Lambda}(\theta)$ immediately follows from the fact that the boundary conditions in (2.3.13) are linearly independent and symmetric, [158], Theorem XII.4.30). The spectrum of $-\Delta_{\alpha,\Lambda}(\theta)$ (cf. Figure 37) is described in

Theorem 2.3.1. *Let $-\infty < \alpha \leq \infty$, $\theta \in [-b/2, b/2)$. Then the essential spectrum of $-\Delta_{\alpha,\Lambda}(\theta)$ is empty,*

$$\sigma_{\mathrm{ess}}(-\Delta_{\alpha,\Lambda}(\theta)) = \varnothing \tag{2.3.14}$$

and thus the spectrum of $-\Delta_{\alpha,\Lambda}(\theta)$ is purely discrete. In particular, its eigenvalues $E_m^{\alpha,\Lambda}(\theta)$, $m \in \mathbb{N}$ (ordered in magnitude) are given by

$$E_m^{\alpha,\Lambda}(\theta) = [k_m^{\alpha,\Lambda}(\theta)]^2, \qquad m \in \mathbb{N}, \tag{2.3.15}$$

where $k_m^{\alpha,\Lambda}(\theta)$, $m \in \mathbb{N}$, are the solutions of the Kronig–Penney relation

$$\cos(\theta a) = \cos(ka) + (\alpha/2k)\sin(ka), \qquad \operatorname{Im} k \geq 0. \tag{2.3.16}$$

For $\alpha \in \mathbb{R} - \{0\}$ the corresponding eigenfunctions read

$$g_m^{\alpha,\Lambda}(\theta, v) = C \begin{cases} e^{ik_m^{\alpha,\Lambda}(\theta)v} + e^{i\theta a} e^{-ik_m^{\alpha,\Lambda}(\theta)a} \dfrac{e^{-i\theta a} e^{-ik_m^{\alpha,\Lambda}(\theta)a} - 1}{e^{i\theta a} e^{-ik_m^{\alpha,\Lambda}(\theta)a} - 1} e^{-ik_m^{\alpha,\Lambda}(\theta)v}, \\ \qquad\qquad -a/2 < v \leq 0, \\ e^{-i\theta a} e^{-ik_m^{\alpha,\Lambda}(\theta)a} e^{ik_m^{\alpha,\Lambda}(\theta)v} + \dfrac{e^{-i\theta a} e^{-ik_m^{\theta,\Lambda}(\theta)a} - 1}{e^{i\theta a} e^{-ik_m^{\alpha,\Lambda}(\theta)a} - 1} e^{-ik_m^{\alpha,\Lambda}(\theta)v}, \\ \qquad\qquad 0 \leq v < a/2, \end{cases}$$
$$m \in \mathbb{N}, \quad \theta \in [-b/2, b/2). \tag{2.3.17}$$

In addition, $E_m^{\alpha,\Lambda}(\theta)$, $\alpha \in \mathbb{R} - \{0\}$, $\theta \in [-b/2, b/2)$, *are nondegenerate and*

$$\begin{aligned} &0 < E_1^{\alpha,\Lambda}(0) < E_1^{\alpha,\Lambda}(-b/2) = \pi^2/a^2 < E_2^{\alpha,\Lambda}(-b/2) < E_2^{\alpha,\Lambda}(0) = 4\pi^2/a^2 \\ &\quad < E_3^{\alpha,\Lambda}(0) < E_3^{\alpha,\Lambda}(-b/2) = 9\pi^2/a^2 < E_4^{\alpha,\Lambda}(-b/2) < E_4^{\alpha,\Lambda}(0) = 16\pi^2/a^2 \\ &\quad < E_5^{\alpha,\Lambda}(0) < \cdots, \qquad \alpha > 0, \end{aligned} \tag{2.3.18}$$

$$\begin{aligned} &E_1^{\alpha,\Lambda}(0) < E_1^{\alpha,\Lambda}(-b/2) < E_2^{\alpha,\Lambda}(-b/2) = \pi^2/a^2 < E_2^{\alpha,\Lambda}(0) < E_3^{\alpha,\Lambda}(0) = 4\pi^2/a^2 \\ &\qquad < E_3^{\alpha,\Lambda}(-b/2) < E_4^{\alpha,\Lambda}(-b/2) = 9\pi^2/a^2 < E_4^{\alpha,\Lambda}(0) < E_5^{\alpha,\Lambda}(0) = 16\pi^2/a^2 \\ &\qquad < E_5^{\alpha,\Lambda}(-b/2) < \cdots, \\ &E_1^{\alpha,\Lambda}(0) < 0, \qquad E_1^{\alpha,\Lambda}(-b/2) \begin{cases} <0 & \text{if } -\alpha > 4/a, \\ =0 & \text{if } -\alpha = 4/a, \\ >0 & \text{if } -\alpha < 4/a, \end{cases} \qquad \alpha < 0. \end{aligned} \tag{2.3.19}$$

All nonconstant eigenvalues $E_m^{\alpha,\Lambda}(\theta)$, $\theta \in [-b/2, b/2)$, $m \in \mathbb{N}$, *are strictly increasing in* $\alpha \in \mathbb{R}$.

For $\alpha = 0$ *the eigenvalues and eigenfunctions explicitly read*

$$\begin{aligned} &E_{m\pm}^{0,\Lambda}(\theta) = \{\pm\theta + [2(m-1)\pi/a]\}^2, \qquad \theta \in (-b/2, 0), \quad m \in \mathbb{N}, \\ &E_m^{0,\Lambda}(0) = [2(m-1)\pi/a]^2, \quad E_m^{0,\Lambda}(-b/2) = [(2m-1)\pi/a]^2, \quad m \in \mathbb{N}, \\ &g_{m\pm}^{0,\Lambda}(\theta, v) = Ce^{i\{\pm\theta + [2(m-1)\pi/a]\}v}, \qquad \theta \in (-b/2, 0), \quad m \in \mathbb{N}, \\ &g_m^{0,\Lambda}(0, v) = C\begin{cases} \cos[2(m-1)\pi v/a], & m \in \mathbb{N}, \\ \sin[2(m-1)\pi v/a], & m = 2, 3, \ldots, \end{cases} \\ &g_m^{0,\Lambda}(-b/2, v) = C\begin{cases} \cos[(2m-1)\pi v/a], \\ \sin[(2m-1)\pi v/a], & m \in \mathbb{N}, \end{cases} \end{aligned} \tag{2.3.20}$$

(note that they are only degenerate for $\theta = -b/2$, $m \in \mathbb{N}$, *and* $\theta = 0$, $m \geq 2$*). For* $\alpha = \infty$ *the Dirichlet boundary condition at zero implies simple eigenvalues (independent of* θ*)*

$$\begin{aligned} &E_m^{\infty,\Lambda} = m^2\pi^2/a^2, \\ &g_m^{\infty,\Lambda}(\theta, v) = C\sin(m\pi v/a)\begin{cases} 1, & -a/2 < v \leq 0, \\ (-1)^m e^{-i\theta a}, & 0 \leq v < a/2, \end{cases} \qquad m \in \mathbb{N}. \end{aligned} \tag{2.3.21}$$

PROOF. Since a is finite, $-\Delta_{\alpha,\Lambda}(\theta)$ has a compact resolvent which proves (2.3.14). The results (2.3.15)–(2.3.17) and (2.3.20), (2.3.21) follow from straightforward computations such that it suffices to discuss the nondegeneracy statement and (2.3.18) and (2.3.19). For $\theta \in (-b/2, 0) \cup (0, b/2)$ and $\alpha \in \mathbb{R}$, $E_m^{\alpha,\Lambda}(\theta)$ is nondegenerate since if $\psi_1(\theta)$ solves $-\psi'' = E\psi$ for some $E \in \mathbb{R}$ and satisfies the boundary condition in (2.3.13), then $\psi_2(-\theta) = \overline{\psi_1(\theta)}$ solves the same equation but different boundary conditions with θ replaced by $-\theta$ (this is also connected with the fact that $-\Delta_{\alpha,\Lambda}(\theta)$ and $-\Delta_{\alpha,\Lambda}(-\theta)$ are antiunitarily equivalent under complex conjugation). Since there are at most two linearly independent solutions of $-\psi'' = E\psi$, $E_m^{\alpha,\Lambda}(\theta)$ is simple. The cases $\theta = 0, -b/2$ are more involved. Thus we consider solutions of

$$\pm 1 = \cos(ka) + (\alpha/2k)\sin(ka), \qquad \operatorname{Im} k \geq 0. \tag{2.3.22}$$

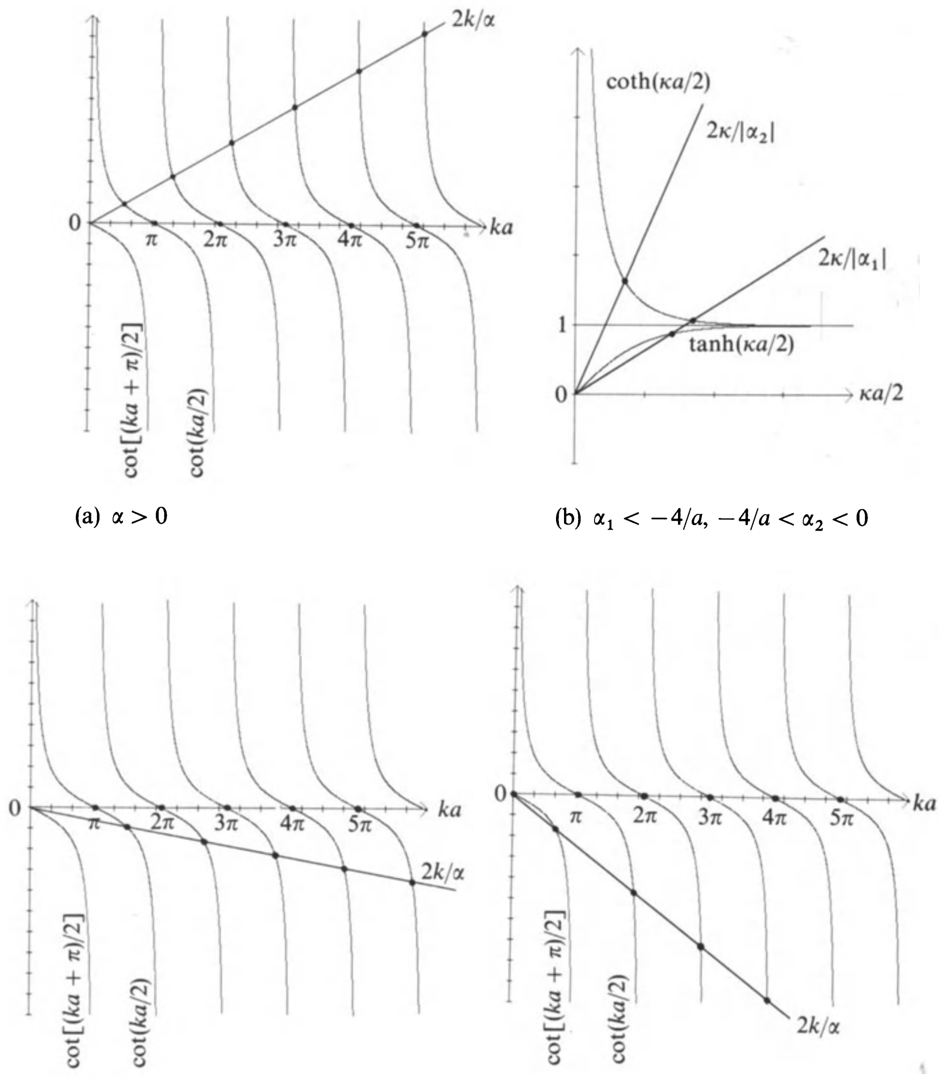
We start with $\alpha > 0$: Let $k = i\kappa$, $\kappa \geq 0$. Then

$$\pm 1 = \cosh(\kappa a) + (\alpha/2\kappa)\sinh(\kappa a) \tag{2.3.23}$$

has obviously no solutions implying that all solutions k of (2.3.22) obey $k^2 > 0$. But for $k > 0$ solutions of (2.3.22) are equivalent to solutions of

$$\begin{aligned} \sin(ka/2) = 0 \quad &\text{or} \quad \cot(ka/2) = 2k/\alpha \quad &&\text{for} \quad \theta = 0, \\ \sin[(ka + \pi)/2] = 0 \quad &\text{or} \quad \cot[(ka + \pi)/2] = 2k/\alpha \quad &&\text{for} \quad \theta = -b/2, \end{aligned} \tag{2.3.24}$$

which now are simple to realize graphically (cf. Figure 35(a)) since $\cot(ka/2)$ (resp. $\cot[(ka + \pi)/2]$) decreases monotonically from $+\infty$ to 0 for k in the



(a) $\alpha > 0$ (b) $\alpha_1 < -4/a$, $-4/a < \alpha_2 < 0$

(c) $\alpha < -4/a$ (d) $-4/a < \alpha < 0$

Figure 35

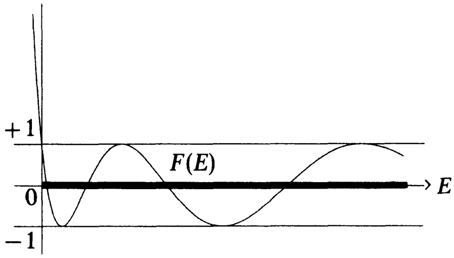
intervals $(m\pi/a, (m+1)\pi/a)$ (resp. $((m+1)\pi/a, (m+2)\pi/a)$), $m = 0, 2, 4, \ldots$. Thus $\cot(ka/2) = 2k/\alpha$ has precisely one solution in each interval $(m\pi/a, (m+1)\pi/a)$, $m = 0, 2, 4, \ldots$, and $m\pi/a$, $(m/2)\pi/a$, $m = 2, 4, \ldots$, are solutions of $\sin(ka/2) = 0$. Applying the same argument to the second line in eq. (2.3.24) we obtain (2.3.18). For $\alpha < 0$ we again take $k = i\kappa$, $\kappa > 0$, and note that (2.3.23) has solutions κ if and only if

$$\begin{aligned} \coth(\kappa a/2) &= 2\kappa/|\alpha| \qquad &&\text{for} \quad \theta = 0, \\ (|\alpha|/2\kappa)\tanh(\kappa a/2) &= 1 \qquad &&\text{for} \quad \theta = -b/2, \end{aligned} \tag{2.3.25}$$

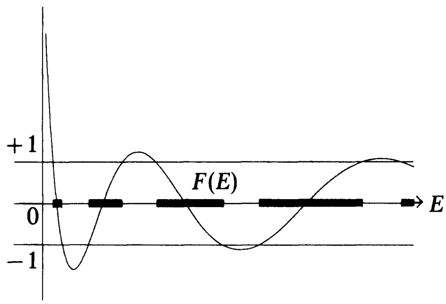
has solutions. Since $\coth(\kappa a/2)$ strictly decreases from $+\infty$ to $+1$ if κ varies in $(0, \infty)$, the equation for $\theta = 0$ has precisely one solution for all $\alpha < 0$ (cf. Figure 35(b)). On the other hand, since $\tanh(\kappa a/2)$ is monotonically increasing from 0 to $+1$ for $\kappa \in [0, \infty)$, the equation for $\theta = -b/2$ has precisely one solution if and only if

$$|\alpha| \geq 4/a, \qquad \alpha < 0. \tag{2.3.26}$$

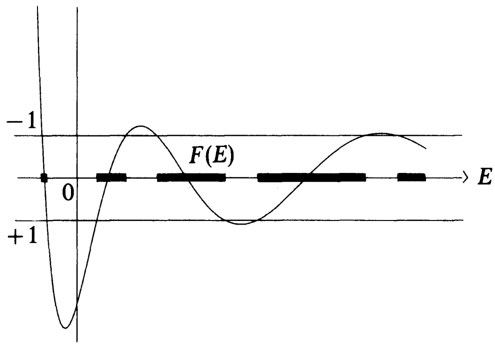
The rest of (2.3.19) now follows from (2.3.24) as described earlier (cf. Figure 35(c), (d)). Simplicity of the eigenvalues for $\theta = 0$, $-b/2$ follows from the calculation leading to (2.3.17). The monotonicity statement after (2.3.19) immediately follows from (2.3.16) and the fact that for $k \geq 0$, $\sin(ka)$ has constant sign whenever the right-hand side of (2.3.16) is strictly decreasing from $+1$ to -1 or strictly increasing from -1 to $+1$. ■



(a) $\alpha = 0$



(b) $\alpha = 20$



(c) $\alpha = -16$

Figure 36 $F(E) = \cos(\sqrt{E}) + (\alpha/2\sqrt{E})\sin(\sqrt{E})$, $\operatorname{Im}\sqrt{E} \geq 0$.

In Figure 36 the right-hand side of the Kronig–Penney relation (2.3.16) is plotted as a function of $E = k^2$ $(a = 1)$, i.e., $F(E) = \cos(\sqrt{E}) + (\alpha/2\sqrt{E})\cdot\sin(\sqrt{E})$. Whenever $F(E) \in [-1, 1]$ fȯr some E we can find a $\theta \in \hat{\Lambda}$ such that the Kronig–Penney relation $F(E) = \cos(\theta)$ is satisfied, and we observe the familar band structure with infinitely many gaps. For a plot of $E_m^{\alpha,\Lambda}(\theta)$, $\alpha > 0$, cf. Figures 37 and 38.

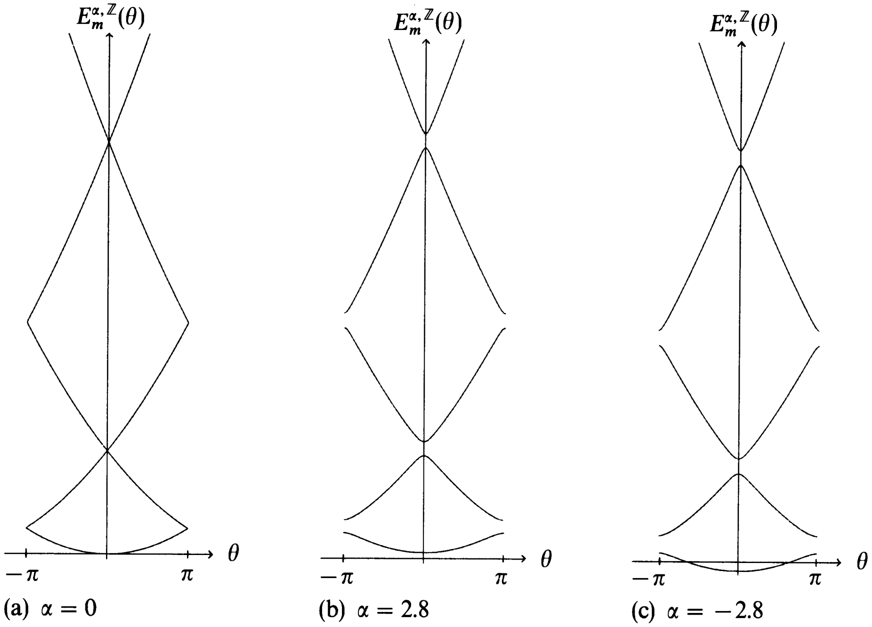


Figure 37 The eigenvalues $E_m^{\alpha,\mathbb{Z}}(\theta) = [k_m^{\alpha,\mathbb{Z}}(\theta)]^2$, $m = 1, \ldots, 4$, of $-\Delta_{\alpha,\mathbb{Z}}(\theta)$ as a function of θ, $-\pi \le \theta < \pi$.

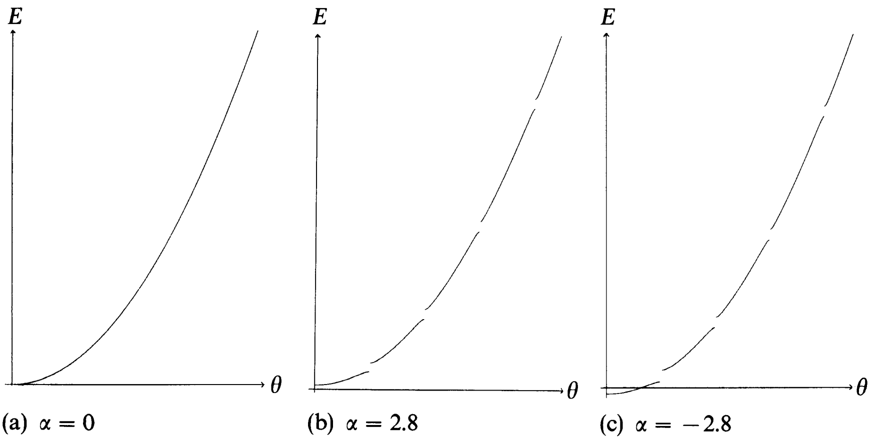


Figure 38 The energy $E = k^2$ as a function of $\theta \ge 0$.

Since $-\Delta_{\alpha,\Lambda}$ commutes with translations implemented by T_a we obtain

Theorem 2.3.2. *Let $-\infty < \alpha \leq \infty$ and $\Lambda = a\mathbb{Z}$, $a > 0$. Then*

$$\tilde{\mathscr{U}}[-\Delta_{\alpha,\Lambda}]\tilde{\mathscr{U}}^{-1} = \int_{[-b/2,b/2)}^{\oplus} \frac{d\theta}{b}[-\Delta_{\alpha,\Lambda}(\theta)]. \tag{2.3.27}$$

PROOF. Let $g_m^{\alpha,\Lambda}(\theta, v)$, $m \in \mathbb{N}$, be the eigenvectors of $-\Delta_{\alpha,\Lambda}(\theta)$ (cf. Theorem 2.3.1) and let

$$\mathscr{D}^{\alpha,\Lambda}(\theta) = [g_m^{\alpha,\Lambda}(\theta), m \in \mathbb{N}] \tag{2.3.28}$$

be the linear span of all eigenvectors of $-\Delta_{\alpha,\Lambda}(\theta)$. Then $\mathscr{D}^{\alpha,\Lambda}(\theta)$ is a core for $-\Delta_{\alpha,\Lambda}(\theta)$. Next we note that (suppressing the α, Λ dependence of g_m for notational convenience)

$$\begin{aligned}(\tilde{\mathscr{U}}^{-1}g_m)(na+) &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}g_m(\theta, 0+)\\ &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}g_m(\theta, 0-) = (\tilde{\mathscr{U}}^{-1}g_m)(na-),\\ &\qquad\qquad n \in Z, \quad m \in \mathbb{N}, \end{aligned}\tag{2.3.29}$$

and by dominated convergence

$$\begin{aligned}(\tilde{\mathscr{U}}^{-1}g_m)'(na+) &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}g_m'(\theta, 0+)\\ &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}[g_m(\theta, 0-) + \alpha g_m(\theta, 0)]\\ &= (\tilde{\mathscr{U}}^{-1}g_m)'(na-) + \alpha(\tilde{\mathscr{U}}^{-1}g_m)(na), \qquad n \in \mathbb{Z}, \quad m \in \mathbb{N}. \end{aligned}\tag{2.3.30}$$

Thus $\tilde{\mathscr{U}}^{-1}g_m$, $m \in \mathbb{N}$, fulfill the boundary conditions in $\mathscr{D}(-\Delta_{\alpha,\Lambda})$. Using dominated convergence once again one infers

$$\begin{aligned}(-\Delta_{\alpha,\Lambda}\tilde{\mathscr{U}}^{-1}g_m)(v + na) &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}(-g_m''(\theta, v))\\ &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}[-\Delta_{\alpha,\Lambda}(\theta)g_m(\theta)](v)\\ &= b^{-1}\int_{-b/2}^{b/2} d\theta\, e^{-in\theta a}E_m^{\alpha,\Lambda}(\theta)g_m(\theta, v),\\ &\qquad n \in \mathbb{Z}, \quad m \in \mathbb{N}, \quad v \in [-a/2, a/2), \end{aligned}\tag{2.3.31}$$

and thus

$$\begin{aligned}(\tilde{\mathscr{U}}[-\Delta_{\alpha,\Lambda}]\tilde{\mathscr{U}}^{-1}g_m)(\theta, v) &= E_m^{\alpha,\Lambda}(\theta)g_m(\theta, v) = [-\Delta_{\alpha,\Lambda}(\theta)g_m(\theta)](v),\\ &\qquad n \in \mathbb{Z}, \quad m \in \mathbb{N}, \quad v \in [-a/2, a/2). \end{aligned}\tag{2.3.32}$$

Since $\mathscr{D}^{\alpha,\Lambda}(\theta)$ is a core for $-\Delta_{\alpha,\Lambda}(\theta)$ the proof is finished. ∎

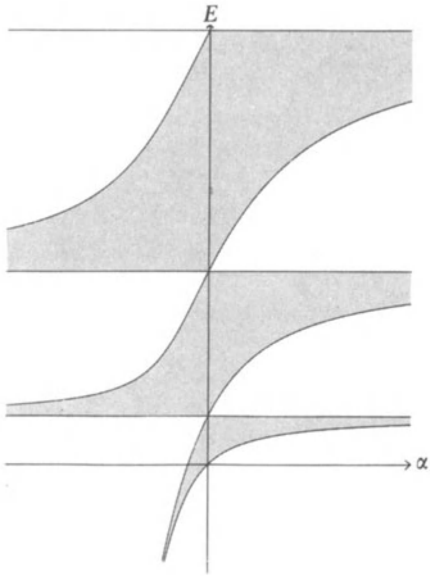


Figure 39 The band spectrum of $-\Delta_{\alpha,\mathbb{Z}}$ as a function of α (cf. also Figures 37 and 38)

The spectrum of $-\Delta_{\alpha,\Lambda}$ (cf. Figure 39) is described in

Theorem 2.3.3. *Let $\alpha \in \mathbb{R}$ and $\Lambda = a\mathbb{Z}$, $a > 0$. Then $-\Delta_{\alpha,\Lambda}$ has a purely absolutely continuous spectrum*

$$\sigma(-\Delta_{\alpha,\Lambda}) = \sigma_{\mathrm{ac}}(-\Delta_{\alpha,\Lambda}) = \bigcup_{m=1}^{\infty} [a_m^{\alpha,\Lambda}, b_m^{\alpha,\Lambda}], \quad a_m^{\alpha,\Lambda} < b_m^{\alpha,\Lambda} \le a_{m+1}^{\alpha,\Lambda}, \quad m \in \mathbb{N},$$

$$\sigma_{\mathrm{sc}}(-\Delta_{\alpha,\Lambda}) = \varnothing, \qquad \sigma_{\mathrm{p}}(-\Delta_{\alpha,\Lambda}) = \varnothing, \tag{2.3.33}$$

where for $\alpha > 0$

$$a_1^{\alpha,\Lambda} > 0, \qquad a_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(0), & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(-b/2), & m \text{ even}, \end{cases} \qquad a_m^{\alpha,\Lambda} > (m-1)^2\pi^2/a^2,$$

$$b_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(-b/2) = m^2\pi^2/a^2, & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(0) = m^2\pi^2/a^2, & m \text{ even}, \end{cases} \qquad m \in \mathbb{N}, \tag{2.3.34}$$

and for $\alpha < 0$

$$a_1^{\alpha,\Lambda} = E_1^{\alpha,\Lambda}(0) < 0, \qquad b_1^{\alpha,\Lambda} = E_1^{\alpha,\Lambda}(-b/2) \begin{cases} <0, & |\alpha| > 4/a, \\ =0, & |\alpha| = 4/a, \\ >0, & |\alpha| < 4/a, \end{cases}$$

$$a_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(0) = (m-1)^2\pi^2/a^2, & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(-b/2) = (m-1)^2\pi^2/a^2, & m \text{ even}, \end{cases}$$

$$b_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(-b/2), & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(0), & m \text{ even}, \end{cases} \qquad m = 2, 3, 4, \ldots, \tag{2.3.35}$$

$$b_m^{\alpha,\Lambda} < m^2\pi^2/a^2, \qquad m \in \mathbb{N},$$

with $E_m^{\alpha,\Lambda}(\theta)$ *the eigenvalues of* $-\Delta_{\alpha,\Lambda}(\theta)$ *described in Theorem* 2.3.1. *As* $m \to \infty$, *the length of the* mth *gap* $a_{m+1}^{\alpha,\Lambda} - b_m^{\alpha,\Lambda}$ *resp. the width of the* mth *band* $b_m^{\alpha,\Lambda} - a_m^{\alpha,\Lambda}$ *asymptotically fulfills*

$$\begin{aligned} a_{m+1}^{\alpha,\Lambda} - b_m^{\alpha,\Lambda} &\underset{m\to\infty}{=} 2|\alpha|a^{-1} + O(m^{-1}), \\ b_m^{\alpha,\Lambda} - a_m^{\alpha,\Lambda} &\underset{m\to\infty}{=} 2m\pi^2a^{-2} - [2|\alpha|a + \pi^2]a^{-2} + O(m^{-1}), \quad \alpha \in \mathbb{R}. \end{aligned} \tag{2.3.36}$$

For $\alpha \in \mathbb{R} - \{0\}$, $-\Delta_{\alpha,\Lambda}$ *has infinitely many gaps in its spectrum (since* $E_m^{\alpha,\Lambda}(0)$, $E_m^{\alpha,\Lambda}(-b/2)$, $m \in \mathbb{N}$, *are simple, all possible gaps in* $\sigma(-\Delta_{\alpha,\Lambda})$ *occur). For* $\alpha = 0$, $-\Delta_{0,\Lambda}$ *equals the kinetic energy operator* $-\Delta$ *on* $H^{2,2}(\mathbb{R})$, *and due to the degeneracy of* $E_m^{0,\Lambda}(0)$, $m \geq 2$, $E_m^{0,\Lambda}(-b/2)$, $m \in \mathbb{N}$, *all gaps close, i.e.,*

$$\sigma_{\text{ess}}(-\Delta_{0,\Lambda}) = \sigma_{\text{ac}}(-\Delta_{0,\Lambda}) = [0, \infty). \tag{2.3.37}$$

For $\alpha = \infty$, $-\Delta_{\infty,\Lambda}$ *equals the Dirichlet Laplacian on* $\mathbb{R} - \Lambda$ *and hence reduces to an infinite direct sum of Dirichlet Laplacians on* $(ma, (m+1)a)$, $m \in \mathbb{Z}$. *As a consequence its spectrum is pure point with each eigenvalue of infinite multiplicity*

$$\begin{aligned} &\sigma_{\text{c}}(-\Delta_{\infty,\Lambda}) = \varnothing, \\ &\sigma_{\text{ess}}(-\Delta_{\infty,\Lambda}) = \sigma_{\text{p}}(-\Delta_{\infty,\Lambda}) = \{m^2\pi^2/a^2 \mid m \in \mathbb{N}\}. \end{aligned} \tag{2.3.38}$$

Furthermore, we note a strict monotonicity of $\sigma(-\Delta_{\alpha,\Lambda})$ *with respect to* α *(being a consequence of the monotonicity of* $E_m^{\alpha,\Lambda}(0)$, $E_m^{\alpha,\Lambda}(-b/2)$, $m \in \mathbb{N}$, *with respect to* $\alpha \in \mathbb{R}$ *as mentioned in Theorem* 2.3.1)

$$\begin{aligned} \sigma(-\Delta_{\alpha,\Lambda}) &\subset \sigma(-\Delta_{\alpha',\Lambda}), \qquad 0 \leq \alpha' < \alpha, \\ \{\sigma(-\Delta_{\alpha,\Lambda}) \cap [0, \infty)\} &\supset \{\sigma(-\Delta_{\alpha',\Lambda}) \cap [0, \infty)\}, \qquad \alpha' < \alpha \leq 0. \end{aligned} \tag{2.3.39}$$

The band edges $a_m^{\alpha,\Lambda}$, $b_m^{\alpha,\Lambda}$, $m \in \mathbb{N}$, *are continuous with respect to* $\alpha \in \mathbb{R}$.

PROOF. Let $\alpha \in \mathbb{R}$. In order to prove the absence of eigenvalues we note that the solutions $k_m^{\alpha,\Lambda}(\theta)$ of (2.3.16) are certainly continuously differentiable with respect to θ. Taking the derivative with respect to θ in (2.3.16) then yields

$$\begin{aligned} -a\sin(\theta a) = &-a[k_m^{\alpha,\Lambda}(\theta)]'\sin[k_m^{\alpha,\Lambda}(\theta)a] \\ &-(\alpha/2)[k_m^{\alpha,\Lambda}(\theta)]^{-2}[k_m^{\alpha,\Lambda}(\theta)]'\sin[k_m^{\alpha,\Lambda}(\theta)a] \\ &+(\alpha/2)[k_m^{\alpha,\Lambda}(\theta)]^{-1}[k_m^{\alpha,\Lambda}(\theta)]'\cos[k_m^{\alpha,\Lambda}(\theta)a], \qquad m \in \mathbb{N}. \end{aligned} \tag{2.3.40}$$

Assuming $[k_m^{\alpha,\Lambda}(\theta_0)]' = 0$ for some $\theta_0 \in (-b/2, 0)$ then yields the contradiction $\sin(\theta_0 a) = 0$. Hence $k_m^{\alpha,\Lambda}(\theta)$ is strictly monotone increasing or decreasing as θ varies in $(-b/2, 0)$. Thus the set $\{\theta \in (-b/2, 0) \mid E_m^{\alpha,\Lambda}(\theta) = E_0\}$, $E_0 \in \mathbb{R}$, has vanishing Lebesgue measure implying (2.3.33) by Theorem XIII.85 of [391]. Absolute continuity of the spectrum follows from [85], Lemmas 10.12–10.15. The general structure of the spectrum in (2.3.33)–(2.3.36) now follows from Theorems 2.3.1 and 2.3.2 and the theory of direct integral decompositions (cf., e.g., [391], Ch. XIII.16). The result (2.3.38) for $\alpha = \infty$ is a direct consequence of (2.3.21).

The asymptotic relation (2.3.36) is obtained as follows. Let, e.g., $\alpha > 0$ and $\tan[\omega(k)] = \alpha/2k$, $k > 0$. Then the band edges are obtained from (2.3.22) by solving

$$(-1)^m \cos[\omega(k)] = \cos[ka - \omega(k)], \qquad k > 0. \tag{2.3.41}$$

The solutions $k_n > 0$ (ordered in magnitude) from $n \geq 2$ on are given by

$$k_{2m}a = m\pi, \qquad k_{2m+1}a = m\pi + 2\omega(k_{2m}), \qquad m \in \mathbb{N}, \tag{2.3.42}$$

such that the mth gap reads

$$(b_m^{\alpha,\Lambda}, a_{m+1}^{\alpha,\Lambda}) = (m^2\pi^2/a^2, (m\pi + 2\omega(k_{2m+1}))^2/a^2). \tag{2.3.43}$$

Since

$$m\pi < k_{2m+1}a = m\pi + 2\omega(k_{2m}) < (m+1)\pi \tag{2.3.44}$$

and

$$\omega(k) = \arctan(\alpha/2k) \underset{k\to\infty}{=} (\alpha/2k) + O(k^{-3}) \tag{2.3.45}$$

one infers (2.3.36). Analogously for $\alpha < 0$. ∎

Given the above result it is simple to compute the density of states of $-\Delta_{\alpha,\Lambda}$ explicitly. In fact, from (2.3.16) we infer

Corollary 2.3.4. *Let $\alpha \in \mathbb{R}$ and $\Lambda = a\mathbb{Z}$, $a > 0$. Then the density of states $d\rho^{\alpha,\Lambda}/dE$ of $-\Delta_{\alpha,\Lambda}$ at a point $E = k^2$ with $E_m^{\alpha,\Lambda}(\theta) = E$, $m \in \mathbb{N}$, is given by*

$$\frac{d\rho^{\alpha,\Lambda}}{dE} = \frac{1}{2\pi k}\frac{d\theta}{dk} = \frac{1}{2\pi|k|}\frac{|\sin(ka)|}{|\sin(\theta a)|}\left\{1 - \alpha\frac{ka\cot(ka) - 1}{2ak^2}\right\},$$

$$\operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad k^2 \in \mathring{\sigma}(-\Delta_{\alpha,\Lambda}), \quad m \in \mathbb{N}, \tag{2.3.46}$$

where $\theta = \theta(k)$ satisfies the Kronig–Penney relation (2.3.16). (Here $\mathring{A}$ denotes the interior of a set $A \subset \mathbb{R}$.) Furthermore, $d\rho^{\alpha,\Lambda}/dE = O(|E - E_m|^{-1/2})$ near the band edges $E_m \in \{a_m^{\alpha,\Lambda}, b_m^{\alpha,\Lambda}\}_{m\in\mathbb{N}}$. As $\alpha \to 0$, $d\rho^{\alpha,\Lambda}/dE$ converges pointwise to the density of states associated with the kinetic energy operator $-\Delta$ on $H^{2,2}(\mathbb{R})$, viz.

$$\frac{d\rho^{\alpha,\Lambda}}{dE} \xrightarrow[\alpha\to 0]{} \frac{d\rho^{0,\Lambda}}{dE} = (2\pi k)^{-1}, \qquad k > 0, \quad E = k^2 \in \mathring{\sigma}(-\Delta_{\alpha_0,\Lambda}). \tag{2.3.47}$$

Proof. Follows from (2.3.16) since

$$\theta(k, \alpha) = (-1)^{m+1}a^{-1}\arccos[\cos(ka) + (\alpha/2k)\sin(ka)] + \begin{cases}(m-1)\pi/a. & m \text{ odd},\\ m\pi/a, & m \text{ even},\end{cases}$$

$$k^2 \in (a_m^{\alpha,\Lambda}, b_m^{\alpha,\Lambda}), \quad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad m \in \mathbb{N}, \tag{2.3.48}$$

where $\arccos(\cdot)$ denotes the principle value. ∎

Bloch waves associated with $-\Delta_{\alpha,\Lambda}$ are derived in Sect. 2.6.

The reader will observe that in contrast to three dimensions (cf. Sect. 1.4) where we gave the whole presentation in p-space, the analysis in one dimension is done completely in x-space. For completeness we will now indicate how one could employ the p-space analysis of Sect. 1.4 in one dimension also.

Consider first the operator in $l^2(\Gamma)$

$$(\hat{H}^\omega(\theta)g)(\gamma) = (\gamma+\theta)^2 g(\gamma) + a^{-1}\mu^\omega(\chi_\omega(\cdot+\theta), g)\chi_\omega(\gamma+\theta), \quad \gamma\in\Gamma,\ \omega>0,$$

$$g \in \mathscr{D}(\hat{H}^\omega(\theta)) = \left\{ g\in l^2(\Gamma) \,\middle|\, \sum_{\gamma\in\Gamma} (\gamma+\theta)^4 |g(\gamma)|^2 < \infty \right\}, \qquad \theta\in\bar{\hat{\Lambda}}, \tag{2.3.49}$$

where

$$\chi_\omega(p) = \begin{cases} 1, & |p|\le\omega, \\ 0, & |p|>\omega, \end{cases} \tag{2.3.50}$$

which is the analog of (1.4.30) in one dimension with $N = 1, y_1 = 0$. By Lemma B.5 the resolvent of $\hat{H}^\omega(\theta)$ reads

$$(\hat{H}^\omega(\theta)-k^2)^{-1} = G_k(\theta) - \left[\frac{a}{\mu^\omega} + (\chi_\omega(\cdot+\theta), G_k(\theta)\chi_\omega(\cdot+\theta))\right]^{-1} \cdot$$
$$\cdot(\overline{G_k(\theta)\chi_\omega(\cdot+\theta)}, \cdot)G_k(\theta)\chi_\omega(\cdot+\theta), \tag{2.3.51}$$

where

$$(G_k(\theta)g)(\gamma) = ((\gamma+\theta)^2-k^2)^{-1}g(\gamma),$$
$$k^2\notin|\Gamma+\theta|^2, \quad \operatorname{Im} k\ge 0, \quad g\in l^2(\Gamma), \quad \theta\in\bar{\hat{\Lambda}}, \quad \gamma\in\Gamma. \tag{2.3.52}$$

The subtle point in the three-dimensional case was the computation of the limit of the factor in front of the rank-one part in (2.3.51) as $\omega\to\infty$. In one dimension this term can easily be computed, viz. ([221], p. 23)

$$(\chi_\omega(\cdot+\theta), G_k(\theta)\chi_\omega(\cdot+\theta))$$
$$= \sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\omega}} \frac{1}{(\gamma+\theta)^2-k^2} \xrightarrow[\omega\to\infty]{} \sum_{\gamma\in\Gamma} \frac{1}{(\gamma+\theta)^2-k^2}$$
$$= \frac{a\sin(ka)}{2k[\cos(ka)-\cos(\theta a)]}, \tag{2.3.53}$$

and hence there is no need to renormalize the coupling constant μ^ω, i.e., we simply choose $\mu^\omega = \alpha$ for all ω. Thus

$$\underset{\omega\to\infty}{\text{n-lim}}\ (\hat{H}^\omega(\theta)-k^2)^{-1}$$
$$\equiv (-\hat{\Delta}_{\alpha,\Lambda}(-\theta)-k^2)^{-1}$$
$$= G_k(\theta) + (\alpha/a)\frac{\cos(ka)-\cos(\theta a)}{\cos(\theta a)-\cos(ka)-(\alpha/2k)\sin(ka)}(\overline{F_k(\theta)}, \cdot)F_k(\theta),$$
$$k^2\in\rho(-\hat{\Delta}_{\alpha,\Lambda}(-\theta)), \quad \operatorname{Im} k\ge 0, \quad \theta\in\bar{\hat{\Lambda}}, \quad -\infty<\alpha\le\infty, \tag{2.3.54}$$

where

$$F_k(\theta)(\gamma) = ((\gamma+\theta)^2-k^2)^{-1}, \qquad k^2\notin|\Gamma+\theta|^2, \quad \operatorname{Im} k\ge 0, \quad \theta\in\bar{\hat{\Lambda}}, \quad \gamma\in\Gamma. \tag{2.3.55}$$

As a byproduct we obtain explicitly the resolvent of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$.

Finally, we would like to illustrate the phenomenon of spectral concentration in connection with transmission probabilities when approximating $-\Delta_{-\pi/2,\pi\mathbb{Z}}$ by N-center Hamiltonians with δ-interactions of strength $-\pi/2$ centered at N equally spaced points of mutual distance π. Figure 40(a)–(e) taken from [397] clearly indicates the formation of gaps in the spectrum of the limiting Hamiltonian $-\Delta_{-\pi/2,\pi\mathbb{Z}}$ associated with vanishing transmission probabilities (cf. also [127]).

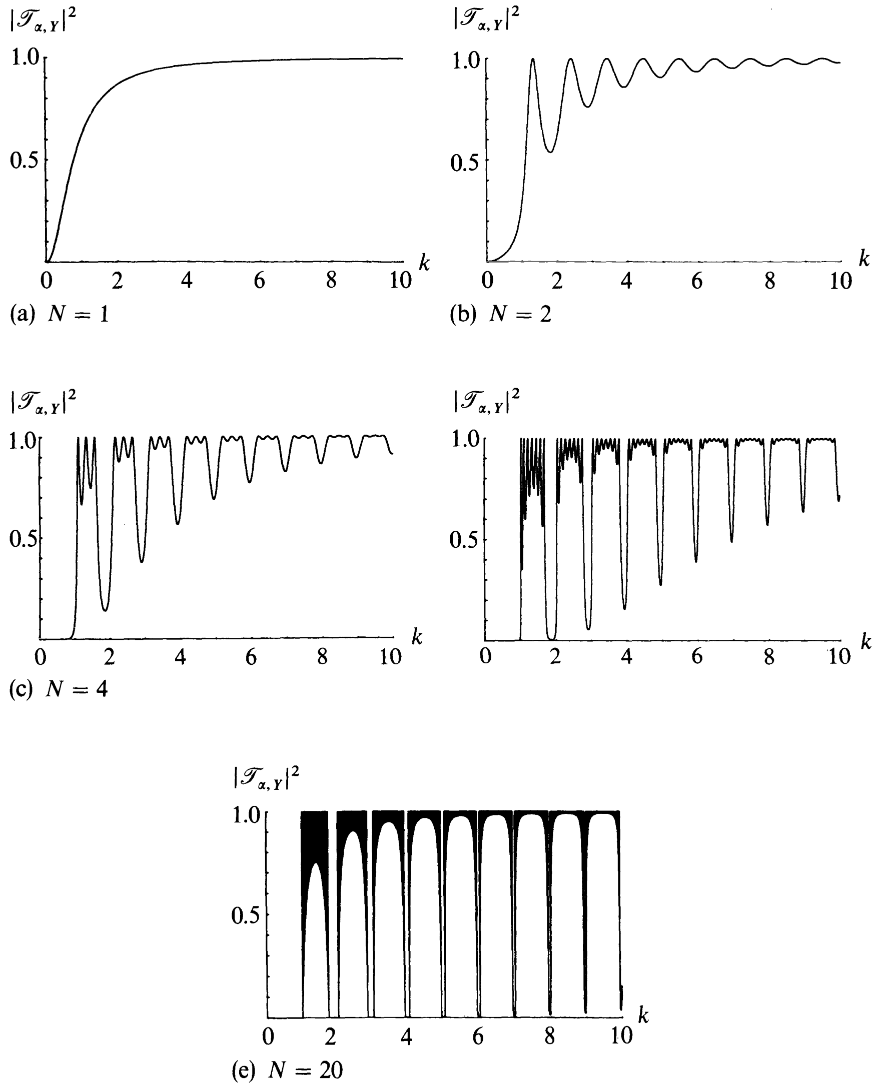


Figure 40 Transmission probability $|\mathscr{T}_{\alpha,Y}(k)|^2$, $k > 0$, for $\alpha = -\pi/2$, $Y = \{y_1, \ldots, y_N\}$, $|y_j - y_{j'}| = \pi, j \neq j', j, j' = 1, \ldots, N$ [397]. Reprinted with the permission of the Society for Industrial and Applied Mathematics from C. Rorres, "Transmission coefficients and eigenvalues of a finite one-dimensional crystal," *SIAM Journal on Applied Mathematics*, Volume 27, Number 2, 1974. All rights reserved. Copyright 1974 by the Society for Industrial and Applied Mathematics.

So far we have discussed the standard approach to the Kronig–Penney model based on direct integral decompositions of the type (2.3.27). For subsequent generalizations of this model spectral results are much quicker obtained by using the discrete operator (2.1.55) mentioned at the end of Sect. 2.1. In particular, for the Kronig–Penney model, (2.1.55) reads

$$\psi_{j+1}(k) + \psi_{j-1}(k) + \mu(k)\psi_j(k) = \varepsilon(k)\psi_j(k),$$
$$\mu(k) = -\alpha k^{-1}\sin(ka), \quad \varepsilon(k) = 2\cos(ka), \quad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}. \tag{2.3.56}$$

This difference equation is solved by the ansatz

$$\psi_j = e^{\pm i\theta a j}, \qquad \operatorname{Im}\theta \geq 0, \quad j \in \mathbb{Z}, \tag{2.3.57}$$

immediately implying the Kronig–Penney relation (2.3.16). We thus get $k^2 \in \sigma(-\Delta_{\alpha,\Lambda})$, $\operatorname{Im} k \geq 0$, $k \neq \pi m/a$, iff a $\theta \in [0, b/2]$ exists such that (2.3.16) is fulfilled. Near the exceptional values $k_m = \pi m/a$, $m \in \mathbb{Z} - \{0\}$, the expression (2.1.50) blows up since the energies $\pi^2 m^2/a^2$, $m \in \mathbb{Z} - \{0\}$, lie at the band edges (cf. (2.3.34) and (2.3.35)). At $k = 0$, formula (2.1.50) ceases to make sense for $\alpha \geq 0$ and for $\alpha \leq -4/a$.

Next we turn to a generalization describing ordered alloys. Let $\alpha^{(p)}$ be a sequence with period $p \in \mathbb{N}$, i.e.,

$$\alpha^{(p)} = \{\alpha_j^{(p)}\}_{j\in\mathbb{Z}}, \qquad \alpha_{j+p}^{(p)} = \alpha_j^{(p)}, \qquad j \in \mathbb{Z}. \tag{2.3.58}$$

Then (2.1.55) becomes

$$\psi_{j+1}(k) + \psi_{j-1}(k) + \mu_j(k)\psi_j(k) = \varepsilon(k)\psi_j(k),$$
$$\mu_j(k) = -\alpha_j^{(p)}k^{-1}\sin(ka), \quad \varepsilon(k) = 2\cos(ka),$$
$$\operatorname{Im} k \geq 0, \quad k \neq \pi m/a, \quad j, m \in \mathbb{Z}, \tag{2.3.59}$$

which can be written as

$$\prod_{j=0}^{p-1} M_j(k)\Phi_0(k) = \Phi_p(k), \qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m/a, \quad m \in \mathbb{Z}, \tag{2.3.60}$$

where $M_j(k)$ and $\Phi_j(k)$ have been defined by (2.1.54) and (2.1.44), respectively. Since $\det[M_j(k)] = 1, j \in \mathbb{Z}$, $\prod_{j=0}^{p-1} M_j(k)$ has eigenvalues $\lambda, \lambda^{-1} \in \mathbb{C}$. By Bloch's theorem or Floquet theory ([160], [334]) $\Phi_p(k) = e^{ip\theta a}\Phi_0(k)$ and the eigenvalues are given by $e^{\pm i\theta pa}$ implying

$$2^{-1}\operatorname{Tr}\left[\prod_{j=0}^{p-1} M_j(k)\right] = \cos(\theta pa), \qquad \operatorname{Im} k \geq 0, \quad \operatorname{Im}\theta \geq 0. \tag{2.3.61}$$

The energy bands are of course obtained from (2.3.61) by checking for which k, $\operatorname{Im} k \geq 0$, $k \neq \pi m/a$, $m \in \mathbb{Z}$, $2^{-1}\operatorname{Tr}[\Pi_{j=0}^{p-1} M_j(k)]$ lies in the interval $[-1, 1]$ (or equivalently for which k a corresponding $\theta(k) \in [0, \pi/pa]$ exists).

It turns out that the product

$$\mathscr{M}_m(k) = \prod_{j=0}^{m-1} M_j(k), \qquad m \in \mathbb{N}, \tag{2.3.62}$$

can be recursively computed in terms of certain Sturm–Liouville polynomials $P_m(\varepsilon, \mu_0, \ldots, \mu_m)$, $Q_m(\varepsilon, \mu_1, \ldots, \mu_m)$, $m = -1, 0, 1, 2, \ldots$. In fact,

$$\mathscr{M}_m = \begin{bmatrix} P_{m-1} & -Q_{m-1} \\ P_{m-2} & -Q_{m-2} \end{bmatrix}, \qquad m \in \mathbb{N}, \tag{2.3.63}$$

where

$$\begin{aligned} &P_{-1} = 1, \qquad P_0 = \varepsilon - \mu_0, \\ &P_m = (\varepsilon - \mu_m)P_{m-1} - P_{m-2}, \end{aligned} \tag{2.3.64}$$

$$\begin{aligned} &Q_{-1} = 0, \qquad Q_0 = 1, \\ &Q_m = (\varepsilon - \mu_m)Q_{m-1} - Q_{m-2}, \qquad m \in \mathbb{N}. \end{aligned} \tag{2.3.65}$$

In particular, the density of states $d\rho^{\alpha(p),\Lambda}/dE$ of $-\Delta_{\alpha(p),\Lambda}$ at a point $E = k^2$ in the mth band $E_m^{\alpha(p),\Lambda}(\theta) = E$, $m \in \mathbb{N}$, of such models is given by the simple expression

$$\frac{d\rho^{\alpha(p),\Lambda}}{dE} = \frac{1}{2\pi k}\frac{d\theta}{dk} = \frac{(-1)^{m+1}}{4\pi p a k}\frac{d}{dk}\arccos\left\{\mathrm{Tr}\left[\prod_{j=0}^{p-1} M_j(k)\right]\right\},$$
$$\operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad k^2 \in \mathring{\sigma}(-\Delta_{\alpha(p),\Lambda}), \quad m \in \mathbb{N}. \tag{2.3.66}$$

We discuss some special cases. First, let

$$p = 2, \qquad \alpha_j^{(2)} = (-1)^j \alpha, \qquad \alpha \in \mathbb{R}, \quad j \in \mathbb{Z}. \tag{2.3.67}$$

Then (2.3.61) yields the spectral condition

$$\cos^2(\theta a) = \cos^2(ka) - (\alpha/2k)^2 \sin^2(ka), \quad \operatorname{Im} k \geq 0, \ \theta \in [-b/2, b/2). \tag{2.3.68}$$

More generally, taking

$$p = 2, \qquad \alpha_0^{(2)} = \alpha, \qquad \alpha_1^{(2)} = \beta, \qquad \alpha, \beta \in \mathbb{R}, \tag{2.3.69}$$

(2.3.61) implies for the spectrum

$$\cos^2(\theta a) = [\cos(ka) + (\alpha/2k)\sin(ka)][\cos(ka) + (\beta/2k)\sin(ka)],$$
$$\operatorname{Im} k \geq 0, \quad \theta \in [-b/2, b/2). \tag{2.3.70}$$

Next we consider a case which models a certain *superlattice* structure

$$\begin{aligned} &\alpha_j^{(p)} = \begin{cases} \gamma_1, & 0 \leq j \leq p_1 - 1, \\ \gamma_2, & p_1 \leq j \leq p_1 + p_2 - 1, \quad \gamma_1 \neq \gamma_2, \quad \gamma_1, \gamma_2 \in \mathbb{R}, \end{cases} \\ &\alpha_{j+p}^{(p)} = \alpha_j^{(p)}, \qquad p = p_1 + p_2, \quad p_1, p_2 \in \mathbb{N}, \quad j \in \mathbb{Z}. \end{aligned} \tag{2.3.71}$$

Then the matrix $\mathscr{M}_p$ splits into a product of two matrices $\mathscr{M}_{p_1}$ and $\mathscr{M}_{p_2}$ which are associated with the constant sequence γ_1 and γ_2 and with Chebyshev polynomials, respectively. Abbreviating

$$2\cos\phi_l = 2\cos(ka) + \gamma_l k^{-1}\sin(ka), \qquad \operatorname{Im} k \geq 0, \quad \operatorname{Im} \phi_l \geq 0, \quad l = 1, 2, \tag{2.3.72}$$

one gets from (2.3.64) and (2.3.65) (cf. [1], p. 782)

$$P_{m-1}^{(p_l)} = Q_m^{(p_l)} = U_m(\cos\phi_l) = \frac{\sin[(m+1)\phi_l]}{\sin\phi_l}, \qquad m \in \mathbb{N}_0, \quad l = 1, 2, \quad (2.3.73)$$

that

$$\mathcal{M}_p = \mathcal{M}_{p_2}\mathcal{M}_{p_1}$$
$$= \begin{bmatrix} \dfrac{\sin[(p_2+1)\phi_2]}{\sin\phi_2} & -\dfrac{\sin(p_2\phi_2)}{\sin\phi_2} \\ \dfrac{\sin(p_2\phi_2)}{\sin\phi_2} & -\dfrac{\sin[(p_2-1)\phi_2]}{\sin\phi_2} \end{bmatrix} \begin{bmatrix} \dfrac{\sin[(p_1+1)\phi_1]}{\sin\phi_1} & -\dfrac{\sin(p_1\phi_1)}{\sin\phi_1} \\ \dfrac{\sin(p_1\phi_1)}{\sin\phi_1} & -\dfrac{\sin[(p_1-1)\phi_1]}{\sin\phi_1} \end{bmatrix} \quad (2.3.74)$$

which implies by (2.3.61)

$$\begin{aligned} 2\sin\phi_1\sin\phi_2\cos(\theta pa) &= \sin[(p_1+1)\phi_1]\sin[(p_2+1)\phi_2] \\ &\quad - 2\sin(p_1\phi_1)\sin(p_2\phi_2) \\ &\quad + \sin[(p_1-1)\phi_1]\sin[(p_2-1)\phi_2], \\ &\qquad \theta \in [-b/2, b/2). \quad (2.3.75) \end{aligned}$$

Other examples, taking, e.g., different periods a, b, c, $\ldots$, $a \neq b$, $a \neq c$, $b \neq c, \ldots$, and different strengths $\alpha, \beta, \gamma, \ldots$ of the interactions are now obtained in a straightforward manner from (2.1.55).

We conclude this series of examples with an interesting generalization of the *Saxon and Hutner conjecture* concerning gaps in certain "substitutional alloys" described by δ-interactions. The alloy is assumed to consist of $N \in \mathbb{N}$ different sorts of "atoms" represented by equally spaced δ-interactions (with fixed distance $a > 0$ between each other) of strength $\gamma_n \in \mathbb{R}$, $\gamma_n \neq \gamma_{n'}$, $n \neq n'$, n, $n' = 1, \ldots, N$, arranged in the following way: The primitive cell $\hat{\Gamma}$ of the model consists of p_1 points supporting δ-interactions of strength γ_{n_1}, followed by p_2 points supporting δ-interactions of strength γ_{n_2}, up to p_M points supporting δ-interactions of strength γ_{n_M}, $M \geq N$, $M \in \mathbb{N}$. In particular, each γ_n, $n = 1, \ldots, N$, occurs at least once and a finite number of repetitions of blocks with δ-interactions of strength γ_n are allowed. The corresponding model Hamiltonian is then denoted by $-\Delta_{\alpha_p, Y_p + \Lambda_p}$ (cf. Sect. 1.4) where

$$\alpha_p = (\underbrace{\gamma_{n_1}, \ldots, \gamma_{n_1}}_{p_1\text{-times}}, \underbrace{\gamma_{n_2}, \ldots, \gamma_{n_2}}_{p_2\text{-times}}, \ldots, \underbrace{\gamma_{n_M}, \ldots, \gamma_{n_M}}_{p_M\text{-times}}),$$

$$\gamma_n \in \mathbb{R}, \quad \gamma_n \neq \gamma_{n'}, \quad n \neq n', \quad n, n' = 1, \ldots, N, \quad p_l \in \mathbb{N},$$
$$l = 1, \ldots, M, \quad M, N \in \mathbb{N},$$

$$Y_p = \{na \mid 0 \leq n \leq p-1\}, \qquad \Lambda_p = pa\mathbb{Z} = \{npa \mid n \in \mathbb{Z}\}, \quad p = \sum_{l=1}^{M} p_l. \quad (2.3.76)$$

Our main result concerning gaps in the spectrum of $-\Delta_{\alpha_p, Y_p + \Lambda_p}$ then reads

Theorem 2.3.5. *Assume* (2.3.76) *and define* $-\Delta_{\alpha_p, Y_p + \Lambda_p}$ *as described above. Let*

$$\rho_N = \bigcap_{n=1}^{N} \rho(-\Delta_{\gamma_n, a\mathbb{Z}}), \qquad a > 0, \quad N \in \mathbb{N}, \tag{2.3.77}$$

be the intersection of all spectral gaps of the Hamiltonians of the pure Kronig–Penney crystals with potential strength $\gamma_n \in \mathbb{R}$ *and fixed Bravais lattice* $a\mathbb{Z}$, $a > 0$, *modeled by* $-\Delta_{\gamma_n, a\mathbb{Z}}$, $n = 1, \ldots, N$ (*cf.* (2.3.12)). *Then*

$$\rho_N \subseteq \rho(-\Delta_{\alpha_p, Y_p + \Lambda_p}) \qquad \text{for all} \quad p \in \mathbb{N}, \tag{2.3.78}$$

i.e., common spectral gaps of all pure crystals described by $-\Delta_{\gamma_n, a\mathbb{Z}}$, $n = 1, \ldots, N$ *remain spectral gaps for all alloys represented by* $-\Delta_{\alpha_p, Y_p + \Lambda_p}$, $p \in \mathbb{N}$, *consisting of N sorts of atoms.*

PROOF. According to our example discussed in (2.3.71)–(2.3.75) we get

$$\mathscr{M}_p(k) = \prod_{l=1}^{N} \mathscr{M}_{p_l}(k) = \prod_{l=1}^{N} \begin{bmatrix} \sin[(p_l + 1)\phi_l(k)] & -\sin[p_l \phi_l(k)] \\ \sin[p_l \phi_l(k)] & -\sin[(p_l - 1)\phi_l(k)] \end{bmatrix} \frac{1}{\sin[\phi_l(k)]}, \tag{2.3.79}$$

where

$$2\cos[\phi_l(k)] = 2\cos(ka) + \gamma_{n_l} k^{-1} \sin(ka), \qquad \operatorname{Im} k \geq 0, \quad \operatorname{Im} \phi_l \geq 0, \quad l = 1, \ldots, N, \tag{2.3.80}$$

and entries in $\mathscr{M}_{p_l}(k)$ are the Chebyshev polynomials (2.3.73). Energies $k^2 \in \mathbb{R}$ in the spectral gap of all pure crystal Hamiltonians $-\Delta_{\gamma_n, a\mathbb{Z}}$ are now simply characterized by

$$|2\cos(ka) + \gamma_n k^{-1} \sin(ka)| > 2, \qquad \operatorname{Im} k \geq 0 \quad \text{for all} \quad n = 1, \ldots, N, \tag{2.3.81}$$

or equivalently by

$$\phi_l(k) = \begin{cases} i\psi_l(k), \\ i\psi_l(k) + \pi, \end{cases} \qquad \psi_l(k) > 0, \qquad \operatorname{Im} k \geq 0, \quad l = 1, \ldots, N. \tag{2.3.82}$$

Thus in order to prove (2.3.78) it suffices to show that (2.3.82) for some fixed k, $\operatorname{Im} k \geq 0$, implies for all $p \in \mathbb{N}$

$$|\operatorname{Tr}[\mathscr{M}_p(k)]| = \left| \operatorname{Tr}\left[\prod_{l=1}^{N} \mathscr{M}_{p_l}(k) \right] \right| > 2. \tag{2.3.83}$$

It suffices to delete the absolute values in (2.3.81) and (2.3.83) (i.e., to choose $\phi_l(k) = i\psi_l(k)$). This case is now proved as follows. Let

$$M(a_j, b_j, c_j) = \begin{bmatrix} a_j + c_j & -b_j \\ b_j & -a_j + c_j \end{bmatrix}, \qquad a_j > |b_j| \geq 0, \quad c_j \geq 0, \quad j \in \mathbb{N}, \tag{2.3.84}$$

and

$$M(a_j, b_j) = M(a_j, b_j, 0), \qquad a_j > |b_j| \geq 0, \quad j \in \mathbb{N}. \tag{2.3.85}$$

In a first step we show that

$$\operatorname{Tr}\left[\prod_{j=1}^{N} M(a_j, b_j)\right] \geq 0, \qquad N \in \mathbb{N}. \tag{2.3.86}$$

For this purpose we note that

$$M(a_1, b_1)M(a_2, b_2) = \begin{bmatrix} a_1 a_2 - b_1 b_2 & a_2 b_1 - a_1 b_2 \\ a_2 b_1 - a_1 b_2 & a_1 a_2 - b_1 b_2 \end{bmatrix} = \begin{bmatrix} A & B \\ B & A \end{bmatrix} \tag{2.3.87}$$

with the properties

$$\begin{aligned} A &> 0, \\ A \pm B &= (a_1 \pm b_1)(a_2 \mp b_2) > 0. \end{aligned} \tag{2.3.88}$$

Next, we prove by induction that $A_j > 0$, $A_j \pm B_j > 0, j = 1, \ldots, N$, implies

$$\prod_{j=1}^{N} \begin{bmatrix} A_j & B_j \\ B_j & A_j \end{bmatrix} = \begin{bmatrix} C_N & D_N \\ D_N & C_N \end{bmatrix}, \qquad C_N > 0, \quad C_N \pm D_N > 0, \quad N \in \mathbb{N}. \tag{2.3.89}$$

Obviously, (2.3.89) is valid for $N = 1$. Assuming (2.3.89) to be correct for $N \in \mathbb{N}$ we infer

$$\begin{aligned} \prod_{l=1}^{N+1} \begin{bmatrix} A_j & B_j \\ B_j & A_j \end{bmatrix} &= \begin{bmatrix} C_N & D_N \\ D_N & C_N \end{bmatrix} \begin{bmatrix} A_{N+1} & B_{N+1} \\ B_{N+1} & A_{N+1} \end{bmatrix} \\ &= \begin{bmatrix} C_N A_{N+1} + D_N B_{N+1} & C_N B_{N+1} + D_N A_{N+1} \\ C_N B_{N+1} + D_N A_{N+1} & C_N A_{N+1} + D_N B_{N+1} \end{bmatrix} \\ &\equiv \begin{bmatrix} C_{N+1} & D_{N+1} \\ D_{N+1} & C_{N+1} \end{bmatrix}. \end{aligned} \tag{2.3.90}$$

Since

$$\begin{aligned} C_{N+1} \pm D_{N+1} &= (A_{N+1} \pm B_{N+1})(C_N \pm D_N) > 0, \\ C_{N+1} &= [(C_{N+1} + D_{N+1})/2] + [(C_{N+1} - D_{N+1})/2] > 0, \end{aligned} \tag{2.3.91}$$

we get (2.3.89). Taking N even, $N = 2n$, $n \in \mathbb{N}$, we infer

$$\begin{aligned} \operatorname{Tr}\left[\prod_{j=1}^{N} M(a_j, b_j)\right] &= \operatorname{Tr}\{[M(a_1, b_1)M(a_2, b_2)] \cdot \ldots \cdot [M(a_{2n-1}, b_{2n-1})M(a_{2n}, b_{2n})]\} \\ &= \operatorname{Tr}\left\{\prod_{j=1}^{n} \begin{bmatrix} A_j & B_j \\ B_j & A_j \end{bmatrix}\right\} = \operatorname{Tr}\left\{\begin{bmatrix} C_n & D_n \\ D_n & C_n \end{bmatrix}\right\} = 2C_n > 0, \end{aligned} \tag{2.3.92}$$

whereas for N odd, $N = 2n + 1$, $n \in \mathbb{N}$, we get

$$\operatorname{Tr}\left[\prod_{j=1}^{N} M(a_j, b_j)\right] = \operatorname{Tr}\left\{\begin{bmatrix} C_n & D_n \\ D_n & C_n \end{bmatrix}\begin{bmatrix} a_{2n+1} & -b_{2n+1} \\ b_{2n+1} & -a_{2n+1} \end{bmatrix}\right\} = 0. \tag{2.3.93}$$

This proves (2.3.86). In the second step we now show that

$$\operatorname{Tr}\left[\prod_{j=1}^{N} M(a_j, b_j, c_j)\right] \geq 2 \prod_{j=1}^{N} c_j, \qquad N \in \mathbb{N}. \tag{2.3.94}$$

Define

$$f_N(c_1, \ldots, c_N) = \operatorname{Tr}\left[\prod_{j=1}^{N} M(a_j, b_j, c_j)\right], \qquad N \in \mathbb{N}, \tag{2.3.95}$$

then

$$\frac{\partial f_N}{\partial c_j} = f_{N-1}(c_1, \ldots, c_{j-1}, c_{j+1}, \ldots, c_N). \tag{2.3.96}$$

Hence

$$\begin{aligned} f_N(c_1, \ldots, c_N) &= f_N(0, c_2, \ldots, c_N) + \int_0^{c_1} dt \frac{\partial f_N}{\partial t}(t, c_2, \ldots, c_N) \\ &= f_N(0, c_2, \ldots, c_N) + \int_0^{c_1} dt\, f_{N-1}(c_2, \ldots, c_N) \\ &\;\vdots \\ &= c_1 f_{N-1}(c_2, \ldots, c_N) + f_N(0, 0, \ldots, 0) + c_2 f_{N-1}(0, c_3, \ldots, c_N) \\ &\quad + c_3 f_{N-1}(0, 0, c_4, \ldots, c_N) + \cdots + c_N f_{N-1}(0, 0, \ldots, 0). \end{aligned} \tag{2.3.97}$$

Iterating the above procedure, observing (2.3.86) (i.e., $f_N(0, \ldots, 0) \geq 0$ for all $N \in \mathbb{N}$) we obtain

$$f_N(c_1, \ldots, c_N) \geq \prod_{j=1}^{N-1} c_j \operatorname{Tr}\begin{bmatrix} c_N & 0 \\ 0 & c_N \end{bmatrix} = 2 \prod_{j=1}^{N} c_j \tag{2.3.98}$$

and hence (2.3.94). Finally, identifying

$$\begin{aligned} a_l &= \sinh[p_l \psi_l(k)] \cosh[\psi_l(k)]/\sinh[\psi_l(k)], \\ b_l &= \sinh[p_l \psi_l(k)]/\sinh[\psi_l(k)], \\ c_l &= \cosh[p_l \psi_l(k)], \qquad l = 1, \ldots, N, \end{aligned} \tag{2.3.99}$$

inequality (2.3.94) and (2.3.82) imply

$$\operatorname{Tr}[\mathcal{M}_p(k)] = \operatorname{Tr}\left[\prod_{l=1}^{N} \mathcal{M}_{p_l}(k)\right] \geq 2 \prod_{l=1}^{N} \cosh[p_l \psi_l(k)] > 2. \tag{2.3.100}$$

■

For an illustration of Theorem 2.3.5 in the diatomic case, see Figure 41 [404].

Using a simple limiting argument we can now extend Theorem 2.3.5 to an arbitrary bounded sequence α (not necessarily periodic) as follows.

Theorem 2.3.6. *Let $\alpha = \{\alpha_j\}_{j \in \mathbb{Z}}$ be a bounded sequence of real numbers, $\Lambda = a\mathbb{Z}$, $a > 0$, and assume $U \subset \mathbb{R}$ to be open. If*

$$U \subseteq \bigcap_{j \in \mathbb{Z}} \rho(-\Delta_{\alpha_j, \Lambda}) \quad \textit{then} \quad U \subseteq \rho(-\Delta_{\alpha, \Lambda}). \tag{2.3.101}$$

PROOF. Define a periodic sequence $\alpha^{(m)}$ by setting

$$\alpha_j^m = \alpha_j, \qquad |j| \leq m, \tag{2.3.102}$$

and extending periodically. Then $\alpha^{(m)}$ has period $2m + 1$ and we next prove that

$$-\Delta_{\alpha^{(m)},\Lambda} \xrightarrow[m\to\infty]{} -\Delta_{\alpha,\Lambda} \tag{2.3.103}$$

in strong resolvent sense. For this purpose, let

$$\phi \in \mathscr{D}_0(-\Delta_{\alpha,\Lambda}) = \{g \in \mathscr{D}(-\Delta_{\alpha,\Lambda}) | \operatorname{supp}(g) \text{ compact}\}. \tag{2.3.104}$$

If m is large enough we have $\operatorname{supp}(\phi) \subset (-m, m)$. Thus $\phi \in \mathscr{D}(-\Delta_{\alpha^{(m)},\Lambda})$. Next set

$$\psi_\pm = (-\Delta_{\alpha,\Lambda} \pm i)\phi = (-\Delta_{\alpha^{(m)},\Lambda} \pm i)\phi. \tag{2.3.105}$$

Then

$$\begin{aligned}[][(-\Delta_{\alpha^{(m)},\Lambda} \pm i)^{-1} - (-\Delta_{\alpha,\Lambda} \pm i)^{-1}]\psi_\pm \\ = (-\Delta_{\alpha^{(m)},\Lambda} \pm i)^{-1}[-\Delta_{\alpha,\Lambda} + \Delta_{\alpha^{(m)},\Lambda}](-\Delta_{\alpha,\Lambda} \pm i)^{-1}\psi_\pm = 0.\end{aligned} \tag{2.3.106}$$

Since $\mathscr{D}_0(-\Delta_{\alpha,\Lambda})$ is a core for $-\Delta_{\alpha,\Lambda}$ (cf. the discussion following (2.1.10)) (2.3.103) results (cf. [388], Theorem VIII.25). Since the spectrum cannot suddenly expand under strong resolvent convergence ([388], Theorem VIII.24) we infer that any open interval $(c, d) \subseteq U$ with $(c, d) \cap \sigma(-\Delta_{\alpha^{(m)},\Lambda}) = \varnothing$ for all $m \in \mathbb{N}$ in fact satisfies $(c, d) \cap \sigma(-\Delta_{\alpha,\Lambda}) = \varnothing$. Since by hypothesis $(c, d) \cap \sigma(-\Delta_{\alpha_j,\Lambda}) = \varnothing$ for all $j \in \mathbb{Z}$, Theorem 2.3.5 implies $(c, d) \cap \sigma(-\Delta_{\alpha^{(m)},\Lambda}) = \varnothing$ for all $m \in \mathbb{N}$ which completes the proof. ■

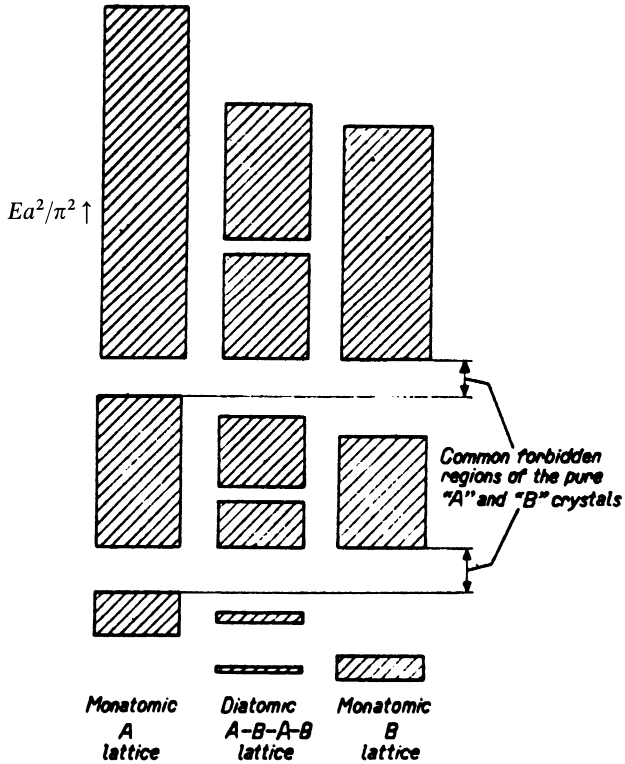


Figure 41 Comparison of energy bands (cross-hatched regions) of a pure A crystal $-\Delta_{A,\Lambda}$, a pure B crystal $-\Delta_{B,\Lambda}$ and the diatomic ... $ABAB$ ... crystal. From Saxon and Hutner, 1949, [404].

Next we derive the analog of Theorem 1.4.6 in the one-dimensional context. Let

$$Y = \{y_1, \ldots, y_N\} \subset \hat{\Gamma}, \qquad \hat{\Gamma} = [-a/2, a/2) \tag{2.3.107}$$

and denote by $-\Delta_{\alpha, Y+\Lambda}$ the analog of (1.4.56), i.e.,

$$-\Delta_{\alpha, Y+\Lambda} = -\frac{d^2}{dx^2},$$

$$\begin{aligned}\mathscr{D}(-\Delta_{\alpha, Y+\Lambda}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - (Y + \Lambda))|\\ g'((y_j + na)+) - g'((y_j + na)-) = \alpha_j g(y_j + na),\\ j = 1, \ldots, N, n \in \mathbb{Z}\},\end{aligned}$$

$$\alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N. \tag{2.3.108}$$

Then we have

Theorem 2.3.7. *Let $\alpha_j \in \mathbb{R}$, $y_j \in \hat{\Gamma}$, $j = 1, \ldots, N$. Then $\sigma(-\Delta_{\alpha, Y+\Lambda}) \cap (-\infty, 0)$ consists of at most N disjoint, closed intervals.*

Proof. Although one could follow the proof of Theorem 1.4.6 step by step we prefer to present another argument which in turn would also apply in the three-dimensional context. Following our earlier arguments in this section (cf. also (1.4.56)) one easily infers that

$$\tilde{\mathscr{U}}[-\Delta_{\alpha, Y+\Lambda}]\tilde{\mathscr{U}}^{-1} = \int_{\hat{\Lambda}}^{\oplus} \frac{d\theta}{b}[-\Delta_{\alpha, \Lambda, Y}(\theta)], \tag{2.3.109}$$

where (cf. (2.3.13))

$$-\Delta_{\alpha, Y, \Lambda}(\theta) = -\frac{d^2}{d\nu^2},$$

$$\begin{aligned}\mathscr{D}(-\Delta_{\alpha, Y, \Lambda}(\theta)) = \{g(\theta) \in H^{2,1}((-a/2, a/2)) \cap H^{2,2}((-a/2, a/2) - Y)|\\ g(\theta, -a/2+) = e^{i\theta a} g(\theta, a/2-), g'(\theta, -a/2+) = e^{i\theta a} g'(\theta, a/2-),\\ g'(\theta, y_j+) - g'(\theta, y_j-) = \alpha_j g(\theta, y_j), j = 1, \ldots, N\},\end{aligned}$$

$$\alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N, \quad \theta \in [-b/2, b/2). \tag{2.3.110}$$

Clearly, $-\Delta_{\alpha, \Lambda, Y}(\theta)$ and $-\Delta_{0, \Lambda, Y}(\theta)$ (i.e., $\alpha_j = 0$, $j = 1, \ldots, N$) are self-adjoint extensions of

$$\dot{H}_Y(\theta) = -\frac{d^2}{d\nu^2},$$

$$\begin{aligned}\mathscr{D}(\dot{H}_Y(\theta)) = \{g(\theta) \in H^{2,2}((-a/2, a/2))|g(\theta, y_j) = 0, j = 1, \ldots, N,\\ g(\theta, -a/2+) = e^{i\theta a} g(\theta, a/2-), g'(\theta, -a/2+) = e^{i\theta a} g'(\theta, a/2-)\},\end{aligned}$$

$$\theta \in [-b/2, b/2). \tag{2.3.111}$$

A simple computation proves that $\dot{H}_Y(\theta)$, $\theta \in [-b/2, b/2)$, has deficiency indices (N, N). Since $-\Delta_{0, \Lambda, Y}(\theta)$, $\theta \in [-b/2, b/2)$ (the free decomposed operator) is obviously nonnegative, $-\Delta_{\alpha,\Lambda,Y}(\theta)$, $\theta \in [-b/2, b/2)$, $\alpha \in \mathbb{R}$, can have at most N negative eigenvalues by Corollary 1 of [494], p. 246. By (2.3.109), $-\Delta_{\alpha,Y+\Lambda}$ has at most N disjoint negative energy bands (cf. (1.4.25)). ∎

Finally, we recall the absence of eigenvalues for periodic systems of the type (2.3.59) and (2.3.60). This implies the irrelevance of the exceptional points $k_m = \pi m/a$, $m \in \mathbb{Z}$, when calculating the spectrum of $-\Delta_{\alpha^{(p)},a\mathbb{Z}}$: Denoting by $h_{\omega^{(p)}}$ the bounded, self-adjoint operator in $l^2(\mathbb{Z})$

$$(h_{\omega^{(p)}}\psi)_j = \psi_{j+1} + \psi_{j-1} + \omega_j^{(p)}\psi_j, \quad p \in \mathbb{N}, \quad j \in \mathbb{Z}, \quad \{\psi_j\}_{j\in\mathbb{Z}} \in l^2(\mathbb{Z}), \tag{2.3.112}$$

where $\omega^{(p)}$ is a sequence of real numbers with period p

$$\omega_{j+p}^{(p)} = \omega_j^{(p)}, \qquad j \in \mathbb{Z}, \tag{2.3.113}$$

we get the standard result

Lemma 2.3.8. *The spectra of $-\Delta_{\alpha^{(p)},a\mathbb{Z}}$ and $h_{\omega^{(p)}}$ are purely continuous, i.e.,*

$$\sigma_p(-\Delta_{\alpha^{(p)},a\mathbb{Z}}) = \varnothing, \qquad \sigma_p(h_{\omega^{(p)}}) = \varnothing. \tag{2.3.114}$$

PROOF. If suffices to discuss $h_{\omega^{(p)}}$. Let $T_{\pm p}$, $p \in \mathbb{N}$, denote the unitary shift operators in $l^2(\mathbb{Z})$

$$(T_{\pm p}\psi)_j = \psi_{j\pm p}, \qquad p \in \mathbb{N}, \qquad \{\psi_j\}_{j\in\mathbb{Z}} \in l^2(\mathbb{Z}). \tag{2.3.115}$$

Then obviously $T_{\pm p}$ commutes with $h_{\omega^{(p)}}$. Assume that e_0 is an eigenvalue of $h_{\omega^{(p)}}$ with corresponding eigenspace $\mathscr{H}_0$. By inspection $T_{\pm p}\mathscr{H}_0 \subseteq \mathscr{H}_0$ implying

$$T_{\pm p}\mathscr{H}_0 = \mathscr{H}_0, \qquad p \in \mathbb{N}, \tag{2.3.116}$$

since $T_{-p} = (T_p)^{-1}$. Thus T_p is reduced by $\mathscr{H}_0$ and $T_p|_{\mathscr{H}_0}$ is unitary. Since $\dim \mathscr{H}_0 \leq 2$, $T_p|_{\mathscr{H}_0}$ has an eigenvalue, i.e.,

$$T_p\phi_0^p = e^{i\delta_0^p}\phi_0^p, \qquad \delta_0^p \in \mathbb{R}, \quad \phi_0^p \in \mathscr{H}_0. \tag{2.3.117}$$

Thus $|\phi_0^p| = \{|\phi_{0j}^p|\}_{j\in\mathbb{Z}}$ is a periodic sequence of period p in $l^2(\mathbb{Z})$ contradicting $|\phi_0^p| \in l^2(\mathbb{Z})$. ∎

Applying Lemmas 10.12–10.14 of [85] one can actually prove that $\sigma(-\Delta_{\alpha^{(p)},a\mathbb{Z}})$ and $\sigma(h_{\omega^{(p)}})$ are purely absolutely continuous.

III.2.4 Half-Crystals

The purpose of this section is to discuss spectral and scattering properties of half-crystals, i.e., models of the type $-\Delta_{\alpha^+,\Lambda^+}$ where

$$\Lambda^+ = \{ja \mid j \in \mathbb{N}_0\}, \qquad \alpha^+ = \{\alpha_j\}_{j\in\mathbb{N}_0}, \qquad \alpha_j = \alpha, \quad \alpha \in \mathbb{R}, \quad j \in \mathbb{N}_0. \tag{2.4.1}$$

Although this model could be analyzed directly, we again prefer the much shorter approach based on the difference equation (2.1.55). Actually, we will treat a more general situation having different half-crystals on the left and right since this problem requires the same amount of work as studying (2.4.1).

Thus we introduce the operator $-\Delta_{\alpha^{-+},\Lambda}$ where

$$\Lambda = a\mathbb{Z}, \qquad a > 0, \qquad \alpha^{-+} = \{\alpha_j\}_{j \in \mathbb{Z}}, \qquad \alpha_j = \begin{cases} \alpha^+, & j = 0, 1, 2, \ldots, \\ \alpha^-, & j = -1, -2, \ldots, \end{cases}$$
$$\alpha^{\pm} \in \mathbb{R}. \quad (2.4.2)$$

(By translations the endpoints $-1, 0$ of the two half-crystals can be shifted to any points $m-1, m, m \in \mathbb{Z}$.) The true half-crystal then corresponds to $\alpha^- = 0$. Concerning spectral properties of $-\Delta_{\alpha^{-+},\Lambda}$ we state

Theorem 2.4.1. *The spectrum of $-\Delta_{\alpha^{-+},\Lambda}$ is purely absolutely continuous and given by*

$$\begin{aligned} \sigma(-\Delta_{\alpha^{-+},\Lambda}) &= \sigma(-\Delta_{\alpha^-,\Lambda}) \cup \sigma(-\Delta_{\alpha^+,\Lambda}), \\ \sigma_{\mathrm{sc}}(-\Delta_{\alpha^{-+},\Lambda}) &= \varnothing, \qquad \sigma_{\mathrm{p}}(-\Delta_{\alpha^{-+},\Lambda}) = \varnothing, \end{aligned} \tag{2.4.3}$$

where $-\Delta_{\alpha^{\pm},\Lambda}$ denote the infinite crystals (i.e., Kronig–Penney models) of strength $\alpha^{\pm}$ and Bravais lattice $\Lambda = a\mathbb{Z}$ (cf. (2.3.12)). On the interior of the set $\sigma(-\Delta_{\alpha^-,\Lambda}) \cap \sigma(-\Delta_{\alpha^+,\Lambda})$ the spectral multiplicity of $-\Delta_{\alpha^{-+},\Lambda}$ equals 2 whereas on $\sigma(-\Delta_{\alpha^{-+},\Lambda}) - \{\sigma(-\Delta_{\alpha^-,\Lambda}) \cap \sigma(-\Delta_{\alpha^+,\Lambda})\}$ the multiplicity is 1.

PROOF. We have to solve (suppressing the k-dependence)

$$\psi_{j+1} + \psi_{j-1} + \mu_j \psi_j = \varepsilon \psi_j, \qquad \psi_j \in \mathbb{C}, \quad j \in \mathbb{Z},$$

$$\varepsilon = 2\cos(ka), \qquad \mu_j = \begin{cases} \mu^+, & j = 0, 1, 2, \ldots, \\ \mu^-, & j = -1, -2, \ldots, \end{cases} \qquad \mu^{\pm} = -\alpha^{\pm} k^{-1} \sin(ka),$$
$$k \neq m\pi/a, \quad m \in \mathbb{Z}. \quad (2.4.4)$$

The ansatz

$$\psi_j^+ = \begin{cases} N_-[e^{i\theta_- aj} + e^{-i\theta_- aj}\mathscr{R}^{\mathrm{l}}], & j = -1, -2, \ldots, \\ N_+ e^{i\theta_+ aj}\tilde{\mathscr{T}}^{\mathrm{l}}, & j = 0, 1, 2, \ldots, \quad \mathrm{Im}\,\theta_{\pm} \geq 0, \end{cases} \tag{2.4.5}$$

in (2.4.4) yields

$$\cos(\theta_{\mp} a) = (\varepsilon - \mu^{\mp})/2, \qquad \mathrm{Im}\,\theta_{\pm} \geq 0, \tag{2.4.6}$$

for $j \leq -2$ and $j \geq 1$, respectively. Here $N_{\mp} \neq 0$ are (k-dependent) normalization constants to be determined later on. At $j = -1$ one obtains

$$N_+ \tilde{\mathscr{T}}^{\mathrm{l}} + N_-[e^{2i\theta_- a} - (\varepsilon - \mu^-)e^{i\theta_- a}]\mathscr{R}^{\mathrm{l}} = N_-[(\varepsilon - \mu^-)e^{-i\theta_- a} - e^{-2i\theta_- a}] \tag{2.4.7}$$

and at $j = 0$ we get

$$N_+[e^{i\theta_+ a} - (\varepsilon - \mu^+)]\tilde{\mathscr{T}}^{\mathrm{l}} + N_- e^{i\theta_- a}\mathscr{R}^{\mathrm{l}} = -N_- e^{-i\theta_- a}. \tag{2.4.8}$$

Similarly, the ansatz

$$\psi_j^- = \begin{cases} M_+[e^{-i\theta_+ aj} + e^{i\theta_+ aj}\mathscr{R}^{\mathrm{r}}], & j = 0, 1, 2, \ldots, \\ M_- e^{-i\theta_- aj}\tilde{\mathscr{T}}^{\mathrm{r}}, & j = -1, -2, \ldots, \quad \mathrm{Im}\,\theta_{\pm} \geq 0, \end{cases} \tag{2.4.9}$$

yields again (2.4.6) for $j \leq -2$ and $j \geq 1$, respectively. For $j = -1$ one infers

$$M_-[e^{2i\theta_- a} - (\varepsilon - \mu^-)e^{i\theta_- a}]\tilde{\mathscr{T}}^{\mathrm{r}} + M_+ \mathscr{R}^{\mathrm{r}} = -M_+ \tag{2.4.10}$$

and for $j = 0$

$$M_- e^{i\theta_- a}\tilde{T}^{\mathrm{r}} + M_+[e^{i\theta_+ a} - (\varepsilon - \mu^+)]\mathscr{R}^{\mathrm{r}} = M_+[(\varepsilon - \mu^+) - e^{-i\theta_+ a}] \quad (2.4.11)$$

results. Here $M_\pm$ are again (k-dependent) normalization factors. Checking the determinant of the system (2.4.7), (2.4.8) shows that there exists a unique solution for $\tilde{T}^{\mathrm{l}}$, $\mathscr{R}^{\mathrm{l}}$ ($\mathscr{R}^{\mathrm{l}} \neq 0$) iff

$$\theta_- \neq -\theta_+. \quad (2.4.12)$$

Similarly, (2.4.10) and (2.4.11) yield a unique solution for $\tilde{T}^{\mathrm{r}}$, $\mathscr{R}^{\mathrm{r}}$ ($\mathscr{R}^{\mathrm{r}} \neq 0$) iff (2.4.12) holds. Next, let h_0 and h denote the bounded and self-adjoint operators in $l^2(\mathbb{Z})$

$$\begin{aligned} (h_0\psi)_j &= \psi_{j+1} + \psi_{j-1}, \\ (h\psi)_j &= (h_0\psi)_j + \mu_j\psi_j, \qquad \{\psi_j\}_{j\in\mathbb{Z}} \in l^2(\mathbb{Z}). \end{aligned} \quad (2.4.13)$$

Then the fact that

$$\sigma(h_0) = \sigma_{\mathrm{c}}(h_0) = [-2, 2], \qquad \sigma_{\mathrm{p}}(h_0) = \varnothing \quad (2.4.14)$$

implies

$$-2 + \min(\mu^-, \mu^+) \leq h \leq 2 + \max(\mu^-, \mu^+). \quad (2.4.15)$$

Consequently, (2.4.6) determines the values of ε in the spectrum of h for real values of $\theta_\pm$. Actually, we may restrict ourselves to

$$\theta_\pm \in [0, \pi/a] \quad (2.4.16)$$

implying

$$\varepsilon \in [-2 + \min(\mu^-, \mu^+), 2 + \max(\mu^-, \mu^+)] = \sigma(h), \quad (2.4.17)$$

since then (2.4.12) is obviously fulfilled for all $\theta_\pm \in (0, \pi/a]$. Rewritten in terms of k this means (cf. Theorems 2.1.5 and 2.3.1)

$$k^2 \in \sigma(-\Delta_{\alpha^-,\Lambda}) \cup \sigma(-\Delta_{\alpha^+,\Lambda}), \qquad \operatorname{Im} k \geq 0, \quad (2.4.18)$$

and hence the first part of (2.4.3) holds. The statements about the multiplicity of the spectrum now simply follow from the linear independence of the two solutions

$$\psi^\pm = \{\psi_j^\pm\}_{j\in\mathbb{Z}} \in l^\infty(\mathbb{Z}) \quad (2.4.19)$$

defined in (2.4.5) and (2.4.9) and the fact that

$$\varepsilon \in (-2 + \max(\mu^-, \mu^+), 2 + \min(\mu^-, \mu^+)) \quad (2.4.20)$$

is equivalent to

$$k^2 \in \{\sigma(-\Delta_{\alpha^-,\Lambda}) \cap \sigma(-\Delta_{\alpha^+,\Lambda})\}^0, \qquad \operatorname{Im} k \geq 0, \quad (2.4.21)$$

(where $\mathring{A}$ denotes the interior of a set $A \subset \mathbb{R}$). The absence of the singular continuous spectrum now follows by mimicking the standard construction of the (absolutely continuous) spectral measure associated with second-order finite difference operators (cf., e.g., [46], [120], [122], [214]). It remains to prove the absence of eigenvalues of $-\Delta_{\alpha^{-+},\Lambda}$. According to (2.1.52) and the remarks after (2.1.55) we only need to show

$$\sigma_{\mathrm{p}}(h) = \varnothing. \quad (2.4.22)$$

Since $\mathscr{R}^{\mathrm{r}}$, $\mathscr{R}^{\mathrm{l}} \neq 0$, $\psi^\pm$ in (2.4.19) is a fundamental set of solutions of $h\psi = \varepsilon\psi$, $\psi \in l^\infty(\mathbb{Z})$, if $\operatorname{Im} \theta_\pm = 0$. But then $\psi^\pm \notin l^2(\mathbb{Z})$ completes the proof. ■

In the special case where $\alpha^- = 0$, (2.4.3) and (2.3.33) imply that the spectrum of the true half-crystal is simply given by $[a_1^{\alpha^+,\Lambda}, b_1^{\alpha^+,\Lambda}] \cup [0, \infty)$.

The multiplicity statements in Theorem 2.4.1 confirm the intuitive ideas that a particle in the left half-crystal moving to the right can only penetrate into the right half-crystal if its energy lies in an allowed band for both infinite crystals (represented by $-\Delta_{\alpha^\pm,\Lambda}$). In that case a particle moving to the left in the right half-crystal with the same energy penetrates into the left half-crystal implying spectral multiplicity two. In the remaining case, where a particle in the left (right) half-crystal runs to the right (left) with an energy lying in a gap of the infinite crystal described by $-\Delta_{\alpha^+,\Lambda}(-\Delta_{\alpha^-,\Lambda})$ one expects total reflection. Thus the transmission coefficient from the left (right) should be zero and hence the reflection coefficient from the left (right) of modulus one implying spectral multiplicity one in this case. These results are actually contained in the following.

Theorem 2.4.2. *Let* $k^2 \in \{\sigma(-\Delta_{\alpha^-,\Lambda}) \cap \sigma(-\Delta_{\alpha^+,\Lambda})\}^0$, $\operatorname{Im} k \geq 0$. *Then the transmission and reflection coefficients from the left and right associated with* $-\Delta_{\alpha^{-+},\Lambda}$ *are given by*

$$\mathcal{T}^{1}_{\alpha^{-+},\Lambda}(k) = \frac{2i \sin^{1/2}[\theta_-(k)a] \sin^{1/2}[\theta_+(k)a]}{e^{i\theta_-(k)a} - e^{-i\theta_+(k)a}} = \mathcal{T}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k), \tag{2.4.23}$$

$$\begin{aligned} \mathcal{R}^{1}_{\alpha^{-+},\Lambda}(k) &= \frac{e^{-i\theta_+(k)a} - e^{-i\theta_-(k)a}}{e^{i\theta_-(k)a} - e^{-i\theta_+(k)a}}, \\ \mathcal{R}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k) &= \frac{e^{i\theta_+(k)a} - e^{i\theta_-(k)a}}{e^{i\theta_-(k)a} - e^{-i\theta_+(k)a}}, \end{aligned} \tag{2.4.24}$$

where (*cf.* 2.3.16))

$$\cos[\theta_\pm(k)a] = \cos(ka) + (\alpha^\pm/2k)\sin(ka), \qquad \theta_\pm(k) \in (0, \pi/a). \tag{2.4.25}$$

In particular, the on-shell scattering matrix in $\mathbb{C}^2$

$$\mathcal{S}_{\alpha^{-+},\Lambda}(k) = \begin{bmatrix} \mathcal{T}^{1}_{\alpha^{-+},\Lambda}(k) & \mathcal{R}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k) \\ \mathcal{R}^{1}_{\alpha^{-+},\Lambda}(k) & \mathcal{T}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k) \end{bmatrix} \tag{2.4.26}$$

is unitary in this case.

If $k^2 \in \{\sigma(-\Delta_{\alpha^{-+},\Lambda}) - \sigma(-\Delta_{\alpha^+,\Lambda})\}^0$, $\operatorname{Im} k \geq 0$, *then*

$$\mathcal{T}^{1}_{\alpha^{-+},\Lambda}(k) = 0, \tag{2.4.27}$$

$$\mathcal{R}^{1}_{\alpha^{-+},\Lambda}(k) = -\frac{e^{\kappa_+(k)a} - e^{-i\theta_-(k)a}}{e^{\kappa_+(k)a} - e^{i\theta_-(k)a}}, \tag{2.4.28}$$

where

$$\begin{aligned} \cos[\theta_-(k)a] &= \cos(ka) + (\alpha^-/2k)\sin(ka), & \theta_-(k) &\in (0, \pi/a) \\ \cosh[\kappa_+(k)a] &= \cos(ka) + (\alpha^+/2k)\sin(ka), & \kappa_+(k) &= -i\theta_+(k) > 0. \end{aligned} \tag{2.4.29}$$

Similarly, if $k^2 \in \{\sigma(-\Delta_{\alpha^{-+},\Lambda}) - \sigma(-\Delta_{\alpha^-,\Lambda})\}^0$, $\operatorname{Im} k \geq 0$, *then*

$$\mathscr{T}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k) = 0, \tag{2.4.30}$$

$$\mathscr{R}^{\mathrm{r}}_{\alpha^{-+},\Lambda}(k) = -\frac{e^{-\kappa_-(k)a} - e^{i\theta_+(k)a}}{e^{-\kappa_-(k)a} - e^{-i\theta_+(k)a}}, \tag{2.4.31}$$

where

$$\begin{aligned} \cos[\theta_+(k)a] &= \cos(ka) + (\alpha^+/2k)\sin(ka), \quad \theta_+(k) \in (0, \pi/a), \\ \cosh[\kappa_-(k)a] &= \cos(ka) + (\alpha^-/2k)\sin(ka), \quad \kappa_-(k) = -i\theta_-(k) > 0. \end{aligned} \tag{2.4.32}$$

Proof. For simplicity we suppress the α^{-+}, Λ dependence in all quantities involved. Because of $\psi(k, aj) = \psi_j(k)$ (cf. (2.1.49)) we only need to solve (2.4.7), (2.4.8) and (2.4.10), (2.4.11). Let $k^2 \in \{\sigma(-\Delta_{\alpha^-,\Lambda}) \cap (-\Delta_{\alpha^+,\Lambda})\}^0$, $\operatorname{Im} k \geq 0$. Then (2.4.24) and

$$\begin{aligned} \tilde{T}^{\mathrm{l}}(k) &= \frac{N_-(k)}{N_+(k)} \frac{e^{i\theta_-(k)a} - e^{-i\theta_-(k)a}}{e^{i\theta_-(k)a} - e^{-i\theta_+(k)a}}, \\ \tilde{T}^{\mathrm{r}}(k) &= \frac{M_+(k)}{M_-(k)} \frac{e^{i\theta_+(k)a} - e^{-i\theta_+(k)a}}{e^{i\theta_-(k)a} - e^{-i\theta_+(k)a}}, \quad \theta_\pm(k) \in (0, \pi/a), \end{aligned} \tag{2.4.33}$$

result. Since the "plane waves" $e^{\pm i\theta_\pm(k)aj}$ in (2.4.5) and (2.4.9) have to be normalized identically we actually infer

$$N_-(k) = M_-(k), \qquad N_+(k) = M_+(k). \tag{2.4.34}$$

Finally, time reversal invariance implies equal transmission coefficients and hence

$$\left[\frac{N_+(k)}{N_-(k)}\right]^2 = \frac{\sin[\theta_-(k)a]}{\sin[\theta_+(k)a]}, \qquad \theta_\pm(k) \in (0, \pi/a). \tag{2.4.35}$$

Insertion of (2.4.35) into (2.4.33) implies (2.4.23) (since $\mathscr{T}^{\mathrm{l}}(k) \equiv \tilde{T}^{\mathrm{l}}(k)$, $\mathscr{T}^{\mathrm{r}}(k) \equiv \tilde{T}^{\mathrm{r}}(k)$ in this case). If $k^2 \in \{\sigma(-\Delta_{\alpha^{-+},\Lambda}) - \sigma(-\Delta_{\alpha^+,\Lambda})\}^0$, $\operatorname{Im} k \geq 0$ the wave ψ^+ in (2.4.5) decays exponentially for $j \geq 1$. Thus we get $\mathscr{T}^{\mathrm{l}}(k) \equiv 0$ in this case. The results (2.4.30) and (2.4.31) are obtained analogously. ■

Clearly, the above results immediately generalize to more complex situations. For example, one could think of gluing together two half-crystals which stem from pure crystal models of the type $-\Delta_{\alpha_p, Y_p + \Lambda_p}$, $-\Delta_{\tilde{\alpha}_q, \tilde{Y}_q + \tilde{\Lambda}_q}$ where $\Lambda_p = pa\mathbb{Z}$, $\tilde{\Lambda}_q = q\tilde{a}\mathbb{Z}$, $a > 0$, $\tilde{a} > 0$, and α_p (resp. $\tilde{\alpha}_q$) have periods $p, q \in \mathbb{N}$ (cf. (2.3.76)). Then Theorem 2.4.1 directly extends to this case and Theorem 2.3.5 can be used to locate gaps in the spectrum of the composed half-crystals.

III.2.5 Quasi-Periodic δ-Interactions

This section is devoted to a brief study of quasi-periodic δ-interactions. Again we rely heavily on the corresponding difference equation approach.

Let $h(\lambda, \theta, \phi)$ denote the following bounded, self-adjoint operator in $l^2(\mathbb{Z})$

$$\begin{aligned} (h(\lambda, \theta, \phi)\psi)_j &= \psi_{j+1} + \psi_{j-1} + \lambda\cos(2\pi j\theta + \phi)\psi_j, \\ j \in \mathbb{Z}, \quad \{\psi_j\}_{j\in\mathbb{Z}} &\in l^2(\mathbb{Z}), \quad \lambda \in \mathbb{R}, \quad \theta \geq 0, \quad \phi \in [0, 2\pi). \end{aligned} \tag{2.5.1}$$

By Theorem 2.1.5 the associated operator in $L^2(\mathbb{R})$ reads $-\Delta_{\gamma(\theta,\phi),\Lambda}$ where $\Lambda = a\mathbb{Z}$, $a > 0$, and $\gamma(\theta, \phi)$ is now of the type

$$\gamma(\theta, \phi) = \{\gamma_j(\theta, \phi)\}_{j\in\mathbb{Z}}, \quad \gamma_j(\theta, \phi) = \gamma\cos(2\pi j\theta + \phi), \qquad j \in \mathbb{Z}, \quad \gamma \in \mathbb{R}. \tag{2.5.2}$$

Moreover, if ε (resp. k^2), $\operatorname{Im} k \geq 0$, denote the energy of $h(\lambda, \theta, \phi)$ (resp. of $-\Delta_{\gamma(\theta,\phi),\Lambda}$), then

$$\varepsilon = 2\cos(ka), \qquad \lambda = -(\gamma/k)\sin(ka), \qquad \operatorname{Im} k \geq 0. \tag{2.5.3}$$

In order to analyze $-\Delta_{\gamma(\theta,\phi),\Lambda}$ we first describe some basic spectral properties of $h(\lambda, \theta, \phi)$. For this purpose we need to recall certan notions in number theory: We call θ a *Liouville number* iff θ is irrational and there are integers $p_n, q_n \xrightarrow[n\to\infty]{} \infty$ with

$$|\theta - (p_n/q_n)| < q_n^{-n}, \qquad n \in \mathbb{N}. \tag{2.5.4}$$

We will also need a subset of Liouville numbers characterized by the fact that there is a $C > 0$ such that

$$|\theta - (p_n/q_n)| \leq Cn^{-q_n}, \qquad n \in \mathbb{N}, \tag{2.5.5}$$

holds. Next, θ is called a *Roth number* iff θ is irrational and for all $\varepsilon > 0$ there is a $C_\varepsilon > 0$ such that for all $p, q \in \mathbb{N}$

$$|\theta - (p/q)| > C_\varepsilon q^{-2-\varepsilon}. \tag{2.5.6}$$

In contrast to Liouville numbers which are of Lebesgue measure zero (but they are dense in $\mathbb{R}$ and uncountable) the set of Roth numbers is of full Lebesgue measure. We also need approximating functions Ω: $[0, \infty) \to (0, \infty)$ of the type

(i) Ω is continuous, decreasing and $\lim_{s\to\infty} \Omega(s) = 0$.
(ii) $-s^{-1}\ln(\Omega(s))$ is decreasing in $s \in (0, \infty)$.
(iii) $-\int_{s_0}^{\infty} ds\, s^{-2}\ln(\Omega(s)) < +\infty$ for any $s_0 > 0$.

A typical example is given by

$$\Omega(s) = \begin{cases} \Omega(s_0), & 0 \leq s \leq s_0 = e^{1+\alpha}, \\ Ce^{-s/(\ln s)^{1+\alpha}}, & s \geq s_0, \quad 0 < \alpha \leq \frac{1}{2}. \end{cases} \tag{2.5.7}$$

Theorem 2.5.1.

(a) *Aubry duality: Fix θ irrational. Then*

$$\sigma(h(\lambda, \theta, \phi)) = (\lambda/2)\sigma(h(4/\lambda, \theta, \phi)), \qquad \lambda \neq 0, \quad \phi \in [0, 2\pi). \tag{2.5.8}$$

(b) *Fix $|\lambda| > 2$ and θ irrational. Then, for a.e. $\phi \in [0, 2\pi)$,*

$$\sigma_{\mathrm{ac}}(h(\lambda, \theta, \phi)) = \varnothing. \tag{2.5.9}$$

If, in addition, θ is a Liouville number obeying (2.5.5) *then, for a.e. $\phi \in [0, 2\pi)$, the spectrum of $h(\lambda, \theta, \phi)$ is purely singular continuous.*

(c) *Let Ω satisfy* (i)–(iii) *above, $\sum_{n=0}^{\infty} \Omega(n) < \frac{1}{4}$ and fix θ to be irrational with* $\inf_{j\in\mathbb{Z}} |s\theta + j| \geq \Omega(s)$ *for all $s > 0$. Then, for $|\lambda|$ small enough and for all $\phi \in [0, 2\pi)$, $h(\lambda, \theta, \phi)$ has some absolutely continuous spectrum which contains a closed set of positive Lebesgue measure.*

(d) *Let Ω satisfy properties* (i)–(iii) *above and fix θ to be irrational with* $\inf_{j\in\mathbb{Z}}|s\theta + j| \geq \Omega(s)$ *for all $s > 0$. Assume, in addition, that θ is a Roth number with continued fraction expansion $\theta = [a_1, a_2, \ldots, a_n, \ldots]$ for which* $\limsup_{n\to\infty} a_n \geq 10$. *Then, for $|\lambda|$ large enough, $h(\lambda, \theta, \phi)$ has for a.e. $\phi \in [0, 2\pi)$ an infinite set of eigenvalues (with exponentially decaying eigenvectors) whose closure has positive Lebesgue measure. If, in addition,* $\limsup_{n\to\infty} a_n = \infty$ *(which happens for a set of θ's with full Lebesgue measure) then, for any $\varepsilon > 0$ there is a $\lambda_0 > 0$ such that for a.e. $\phi \in [0, 2\pi)$ and all $|\lambda| \leq \lambda_0$ (resp. $|\lambda| \geq \lambda_0^{-1}$) the absolutely continuous part of the spectrum (resp. the closure of the set of eigenvalues) of $h(\lambda, \theta, \phi)$ has Lebesgue measure greater than $4 - \varepsilon$ (resp. greater than* $(4 - \varepsilon)\lambda/2$). *(Obviously,* $|\sigma(h(0, \theta, \phi)| = 4$, $|\sigma(h(\lambda, \theta, \phi))| \leq 4 + 2|\lambda|$.)

Given these results and the correspondence (2.5.3) between $h(\lambda, \theta, \phi)$ and $-\Delta_{\gamma(\theta,\phi),\Lambda}$, one can derive corresponding results for $-\Delta_{\gamma(\theta,\phi),\Lambda}$. We state

Theorem 2.5.2.

(a) *Fix θ irrational. Then, for a.e. $\phi \in [0, 2\pi)$, $-\Delta_{\gamma(\theta,\phi),\Lambda}$ has no absolutely continuous spectrum in the region* $\{E = k^2 | \operatorname{Im} k \geq 0, |(\gamma/k)\sin(ka)| > 2\}$. *If, in addition, θ is a Liouville number obeying* (2.5.5) *then, for a.e. $\phi \in [0, 2\pi)$, $\sigma(-\Delta_{\gamma(\theta,\phi),\Lambda})$ is purely singular continuous in that region (provided this region is nonempty).*

(b) *Assume that θ obeys the conditions of Theorem* 2.5.1(c). *Then, for all $\phi \in [0, 2\pi)$, $-\Delta_{\gamma(\theta,\phi),\Lambda}$ has some absolutely continuous spectrum in the region* $\{E = k^2 | \operatorname{Im} k \geq 0, |(\gamma/k)\sin(ka)|$ *small enough*$\}$.

(c) *Assume that θ obeys the conditions of Theorem* 2.5.1(d). *Then, for a.e. $\phi \in [0, 2\pi)$, $-\Delta_{\gamma(\theta,\phi),\Lambda}$ has an infinite set of eigenvalues in the region* $\{E = k^2 | \operatorname{Im} k \geq 0, |(\gamma/k)\sin(ka)|$ *large enough*$\} \cap \sigma(-\Delta_{\gamma(\theta,\phi),\Lambda})$ *(provided the intersection is nonempty).*

The difficulty with Theorem 2.5.2(a) and (c) is that it is not clear whether there exists some spectrum of $-\Delta_{\gamma(\theta,\phi),\Lambda}$ in these regions at all.

III.2.6 Crystals with Defects and Impurity Scattering

We now discuss how to incorporate impurities represented by δ-interactions in the model Hamiltonian $-\Delta_{\alpha,Y}$. In the particular case of the Kronig–Penney Hamiltonian we also discuss scattering on such impurities.

Let $-\Delta_{\alpha,Y}$ be defined as in (2.1.6) and abbreviate by

$$G_{k,\alpha,Y} = (-\Delta_{\alpha,Y} - k^2)^{-1}, \qquad k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k \geq 0, \tag{2.6.1}$$

its resolvent given in (2.1.17). Let $Z \subset \mathbb{R}$ denote the finite set of impurity points

$$Z = \{z_l \in \mathbb{R} | l = 1, \ldots, M\}, \qquad M \in \mathbb{N}, \tag{2.6.2}$$

which support δ-interactions of strength $\gamma_l \in \mathbb{R} - \{0\}$, $l = 1, \ldots, M$. The total

Hamiltonian representing δ-interactions of strength α_j at the points $y_j \in Y$, $j \in J$, and additional δ-interactions of strength γ_l at the impurity points $z_l \in Z$, $l = 1, \ldots, M$, is then denoted by $-\Delta_{\alpha,Y,\gamma,Z}$ where the sequence γ is defined as

$$\gamma = \{\gamma_l \in \mathbb{R} - \{0\} \mid 1 \leq l \leq M\}. \tag{2.6.3}$$

If $z_l \in Z$ equals some $y_j \in Y$ then, depending on whether γ_l equals $-\alpha_j$ or not we get a *defect impurity* (i.e., the vanishing of the δ-interaction at $z_l = y_j$) or a *substitutional impurity* at $z_l = y_j$ when compared to $-\Delta_{\alpha,Y}$. The situation $z_l \notin Y$ describes an *interstitial impurity* at z_l in addition to the system described by $-\Delta_{\alpha,Y}$.

Clearly, $-\Delta_{\alpha,Y,\gamma,Z}$ subordinates to the discussion in Sect. 2.1. Our goal here is to relate spectral properties of $-\Delta_{\alpha,Y,\gamma,Z}$ and $-\Delta_{\alpha,Y}$. As a first result we compare their resolvents:

Theorem 2.6.1. *Let $\alpha_j, \gamma_l \in \mathbb{R} - \{0\}, j \in J, l = 1, \ldots, M$, and assume* (2.1.1). *Suppose that $-\Delta_{\alpha,Y,\gamma,Z}$ and $G_{k,\alpha,Y}$ are defined as above. Then*

$$\begin{aligned}(-\Delta_{\alpha,Y,\gamma,Z} - k^2)^{-1} &\\ = G_{k,\alpha,Y} + \sum_{l,l'=1}^{M} &[\Gamma_{\alpha,Y,\gamma,Z}(k)]_{ll'}^{-1} (\overline{G_{k,\alpha,Y}(z_{l'}, \cdot)}, \cdot) G_{k,\alpha,Y}(\cdot, z_l),\\ &k^2 \in \rho(-\Delta_{\alpha,Y,\gamma,Z}), \quad \operatorname{Im} k \geq 0,\end{aligned} \tag{2.6.4}$$

where

$$\Gamma_{\alpha,Y,\gamma,Z}(k) = [-\gamma_l^{-1}\delta_{ll'} - G_{k,\alpha,Y}(z_l, z_{l'})]_{l,l'=1}^{M}, \quad k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k \geq 0. \tag{2.6.5}$$

PROOF. We first note that both operators $-\Delta_{\alpha,Y,\gamma,Z}$ and $-\Delta_{\alpha,Y}$ are self-adjoint extensions of the closed, symmetric operator in $L^2(\mathbb{R})$

$$\dot{H}_{\alpha,Y,\gamma,Z} = -\frac{d^2}{dx^2},$$

$$\mathscr{D}(\dot{H}_{\alpha,Y,\gamma,Z}) = \{g \in \mathscr{D}(-\Delta_{\alpha,Y}) \mid g(z_l) = 0, z_l \in Z, l = 1, \ldots, M\} \tag{2.6.6}$$

with deficiency indices (M, M). The adjoint of $\dot{H}_{\alpha,Y,\gamma,Z}$ then reads

$$\dot{H}^*_{\alpha,Y,\gamma,Z} = -\frac{d^2}{dx^2},$$

$$\begin{aligned}\mathscr{D}(\dot{H}^*_{\alpha,Y,\gamma,Z}) = \{g \in H^{2,1}(\mathbb{R}) \cap H^{2,2}(\mathbb{R} - \{Y \cup Z\}) |&\\ g'(y_j+) - g'(y_j-) = \alpha_j g(y_j), y_j \in Y - Z, j \in J\}&.\end{aligned} \tag{2.6.7}$$

Since the solutions of the equation

$$\dot{H}^*_{\alpha,Y,\gamma,Z}\psi(k) = k^2\psi(k), \qquad \psi(k) \in \mathscr{D}(\dot{H}^*_{\alpha,Y,\gamma,Z}), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \tag{2.6.8}$$

are given by

$$\psi_l(k, x) = G_{k,\alpha,Y}(x, z_l), \qquad \operatorname{Im} k > 0, \quad z_l \in Z, \quad l = 1, \ldots, M, \tag{2.6.9}$$

the general structure of (2.6.4) follows from Krein's formula (cf. Theorem A.3). The remaining calculations are analogous to that in the proof of Theorem II.2.1.1. ∎

Concerning spectral properties we state

Theorem 2.6.2. *Let $\alpha_j, \gamma_l \in \mathbb{R} - \{0\}, j \in J, l = 1, \ldots, M$, and assume* (2.1.1). *Then*

$$\sigma_{\text{ess}}(-\Delta_{\alpha,Y,\gamma,Z}) = \sigma_{\text{ess}}(-\Delta_{\alpha,Y}). \tag{2.6.10}$$

Moreover, let $(a, b) \subset \rho(-\Delta_{\alpha,Y})$, $-\infty \leq a < b < \infty$. Then $\sigma(-\Delta_{\alpha,Y,\gamma,Z}) \cap (a, b)$ consists of at most M eigenvalues counting multiplicity.

Proof. The invariance of the essential spectrum in (2.6.10) is due to Weyl's theorem ([391], p. 112) and (2.6.4). The rest follows from Corollary 1 in [494], p. 246. ∎

Since a more detailed spectral analysis of $-\Delta_{\alpha,Y,\gamma,Z}$ seems too difficult in general we now specialize to the periodic case and choose Y equal to the lattice $\Lambda = a\mathbb{Z}$, $a > 0$. In addition, we first assume the sequence α to be periodic with period one, i.e., we first investigate impurities in the Kronig–Penney Hamiltonian $-\Delta_{\alpha,\Lambda}$, $\alpha \in \mathbb{R} - \{0\}$ (cf. (2.3.12)).

The following two linearly independent functions

$$\Psi_{\alpha,\Lambda}(k, \sigma, x) = \Psi_{\alpha,\Lambda}(k, \sigma, 0)(\alpha/2k)e^{i\theta\sigma x}e^{-i\theta\sigma x'}\left\{\frac{e^{i\theta\sigma a}\sin(kx') - \sin[k(x' - a)]}{\cos(\theta a) - \cos(ka)}\right\},$$

$$x' = x - a[[x/a]], \quad \operatorname{Im} k \geq 0, \quad \sigma = \pm 1, \quad \operatorname{Im} \theta \geq 0, \quad \operatorname{Re} \theta \geq 0, \tag{2.6.11}$$

where $[[y]]$ denotes the integer part of y (i.e., the largest integer less than or equal to y) and $\theta = \theta(k)$ satisfies the Kronig–Penney relation (2.3.16), solve

$$-\Psi''_{\alpha,\Lambda}(k, \sigma, x) = k^2\Psi_{\alpha,\Lambda}(k, \sigma, x), \quad \operatorname{Im} k \geq 0, \ \sigma = \pm 1, \ x \in \mathbb{R} - \Lambda, \tag{2.6.12}$$

and fulfill the boundary conditions

$$\Psi_{\alpha,\Lambda}(k, \sigma, na+) = \Psi_{\alpha,\Lambda}(k, \sigma, na-),$$
$$\Psi'_{\alpha,\Lambda}(k, \sigma, na+) - \Psi'_{\alpha,\Lambda}(k, \sigma, na-) = \alpha\Psi_{\alpha,\Lambda}(k, \sigma, na),$$
$$\operatorname{Im} k \geq 0, \quad \sigma = \pm 1, \quad n \in \mathbb{N}. \tag{2.6.13}$$

The result (2.6.11) can be quickly derived as follows. Equations (2.6.12) and (2.6.13) yield the homogeneous Lippmann–Schwinger equation

$$\Psi(k, x) = \alpha \sum_{n \in \mathbb{Z}} G_k(x - na)\Psi(k, na) = \alpha \sum_{n \in \mathbb{Z}} G_k(x - na)e^{i\mu na}\Psi(k, 0), \tag{2.6.14}$$

where Bloch's theorem, i.e.,

$$\Psi(k, x + na) = e^{i\mu na}\Psi(k, x), \qquad \operatorname{Im} \mu \geq 0, \quad x \in \mathbb{R}, \quad n \in \mathbb{Z}, \tag{2.6.15}$$

has been used. It remains to evaluate the sum in (2.6.14):

$$\Psi(k, x) = (i\alpha/2k)\Psi(k, 0)\left\{\sum_{n=-\infty}^{[[x/a]]} e^{ikx}e^{i(\mu-k)na} + \sum_{n=[[x/a]]+1}^{\infty} e^{-ikx}e^{i(\mu+k)na}\right\}$$
$$= (i\alpha/2k)\Psi(k, 0)\left\{\frac{e^{i(\mu-k)a[[x/a]]+ikx}}{1-e^{-i(\mu-k)a}} + \frac{e^{i(\mu+k)a([[x/a]]+1)-ikx}}{1-e^{i(\mu+k)a}}\right\}$$
$$= (i\alpha/2k)\Psi(k, 0)e^{i\mu a[[x/a]]}\frac{e^{i\mu a}\sin(kx') - \sin[k(x'-a)]}{\cos(ka) - \cos(\mu a)},$$
$$x' = x - a[[x/a]], \quad x \in \mathbb{R}, \quad \operatorname{Im} k \geq 0, \quad \operatorname{Im} \mu \geq 0. \tag{2.6.16}$$

If $\sigma = +1(-1)$ which corresponds to $\mu > 0$ ($\mu < 0$) in (2.6.16), (2.6.11) represents a wave traveling to the right (left) in the lattice. Moreover, (2.6.11) clearly exhibits Bloch's theorem since $x' = x - a[[x/a]]$ is periodic with the period a of the lattice $\Lambda = a\mathbb{Z}$. We also remark that taking $x = 0$ (i.e., $x' = 0$) in (2.6.11) immediately yields the Kronig–Penney relation (2.3.16).

Now we are prepared to discuss impurities. To avoid too lengthy computations we restrict ourselves to a single impurity at the point $z \in \mathbb{R}$ described by a δ-interaction of strength $\gamma \in \mathbb{R} - \{0\}$. The corresponding Hamiltonian is then denoted by $-\Delta_{\alpha,\Lambda,\gamma,z}$. We start by solving the bound state problem

$$-\Delta_{\alpha,\Lambda,\gamma,z}\Psi_{\alpha,\Lambda,\gamma,z}(k) = k^2\Psi_{\alpha,\Lambda,\gamma,z}(k), \ \Psi_{\alpha,\Lambda,\gamma,z}(k) \in \mathscr{D}(-\Delta_{\alpha,\Lambda,\gamma,z}),$$
$$k^2 \in \mathbb{R}, \quad \operatorname{Im} k \geq 0. \tag{2.6.17}$$

Consequently, $\Psi_{\alpha,\Lambda,\gamma,z}(k, x)$ solves

$$-\psi''(k, x) = k^2\psi(k, x), \qquad x \in R - \{\Lambda \cup \{z\}\}, \tag{2.6.18}$$

with the boundary conditions

$$\psi(k, na+) = \psi(k, na-),$$
$$\psi'(k, na+) - \psi'(k, na-) = \alpha\psi(k, na), \qquad na \in \Lambda - \{z\}, \quad n \in \mathbb{Z}, \tag{2.6.19}$$
$$\psi(k, z+) = \psi(k, z-),$$
$$\psi'(k, z+) - \psi'(k, z-) = [\gamma + \alpha\delta_{z,\Lambda}]\psi(k, z), \tag{2.6.20}$$

where $\delta_{z,\Lambda} = \begin{cases} 1, & z \in \Lambda, \\ 0, & z \notin \Lambda. \end{cases}$ For $x \in \mathbb{R} - \{z\}$, $\psi(k, x)$ also solves $-\Delta_{\alpha,\Lambda}\psi(k) = k^2\psi(k)$. The solutions of (2.6.17) are thus certain linear combinations of $\Psi_{\alpha,\Lambda}(k, \pm 1, x)$. Since $\Psi_{\alpha,\Lambda}(k, \pm 1, x)$ are oscillating for $\theta \in \mathbb{R}$ we need $\operatorname{Im} \theta > 0$ in order to guarantee square integrable solutions. Thus we are led to the ansatz

$$\Psi_{\alpha,\Lambda,\gamma,z}(k, x) = \begin{cases} c_1\dfrac{\Psi_{\alpha,\Lambda}(k, -1, x)}{\Psi_{\alpha,\Lambda}(k, -1, z)}, & x < z, \\[2ex] c_2\dfrac{\Psi_{\alpha,\Lambda}(k, +1, x)}{\Psi_{\alpha,\Lambda}(k, +1, z)}, & x > z, \quad \operatorname{Im} \theta(k) > 0. \end{cases} \tag{2.6.21}$$

Insertion of (2.6.21) into (2.6.20) yields

$$c_1 = c_2 \tag{2.6.22}$$

and

$$c_2 \frac{\Psi'_{\alpha,\Lambda}(k, +1, z+)}{\Psi_{\alpha,\Lambda}(k, +1, z)} - c_1 \frac{\Psi'_{\alpha,\Lambda}(k, -1, z-)}{\Psi_{\alpha,\Lambda}(k, -1, z)} = (\gamma + \alpha\delta_{z,\Lambda})c_1. \tag{2.6.23}$$

Observing

$$\Psi'_{\alpha,\Lambda}(k, \pm 1, z+) - \Psi'_{\alpha,\Lambda}(k, \pm 1, z-) = \alpha\delta_{z,\Lambda}\Psi_{\alpha,\Lambda}(k, \pm 1, z) \tag{2.6.24}$$

(cf. (2.6.12), (2.6.13)) in (2.6.23) we infer

$$c_2 \frac{\Psi'_{\alpha,\Lambda}(k, +1, z\pm)}{\Psi_{\alpha,\Lambda}(k, +1, z)} - c_1 \frac{\Psi'_{\alpha,\Lambda}(k, -1, z\pm)}{\Psi_{\alpha,\Lambda}(k, -1, z)} = \gamma c_1. \tag{2.6.25}$$

Together with (2.6.22) this leads to

$$\begin{aligned} &W(\overline{\Psi_{\alpha,\Lambda}(k, +1)}, \Psi_{\alpha,\Lambda}(k, -1))_{z\pm} \\ &\quad + \gamma \overline{\Psi_{\alpha,\Lambda}(k, +1, z)}\Psi_{\alpha,\Lambda}(k, -1, z) = 0, \end{aligned} \tag{2.6.26}$$

where $W(f, g)_x = \overline{f(x)}g'(x) - \overline{f'(x)}g(x)$ denotes the Wronskian of f and g. With the help of (2.6.11), (2.6.26) simplifies to

$$\begin{aligned} -2ik \sin(\theta a) \sin(ka) + \gamma\{&\sin^2(kz') + \sin^2[k(z' - a)] \\ &- 2\sin(kz')\sin[k(z' - a)]\cos(\theta a)\} = 0, \\ z' = z - a[[z/a]], \quad &\operatorname{Im} k \geq 0, \quad \operatorname{Im} \theta(k) > 0. \end{aligned} \tag{2.6.27}$$

Thus (2.6.27) together with the Kronig–Penney relation (2.3.16) represents the bound state condition. Before we separately discuss the case of substitutional, defect, and interstitial impurities we derive a technical result that enables one to decide in which energy gaps of $-\Delta_{\alpha,\Lambda}$ impurity states associated with $-\Delta_{\alpha,\Lambda,\gamma,z}$ do actually occur:

Lemma 2.6.3. *Let* $k^2 \in (b_m^{\alpha,\Lambda}, a_{m+1}^{\alpha,\Lambda})$, $\operatorname{Im} k \geq 0$, $b_0^{\alpha,\Lambda} = -\infty$, *and suppose that* $K = e^{i\theta a}$ *where* $\theta = (m\pi/a) + i\delta$, $\delta > 0$, $m \in \mathbb{N}_0$, *is a solution of the Kronig–Penney relation* (2.3.16) *such that* $(K + K^{-1})/2 = \cos(ka) + (\alpha/2k)\sin(ka)$. *Assume that* $\psi(k, x)$ *is a real-valued solution of*

$$-\psi''(k, x) = k^2\psi(k, x), \qquad x \in (-a/2, a/2) - \{0\} \tag{2.6.28}$$

satisfying the boundary conditions

$$\begin{aligned} \psi(k, a-) &= K\psi(k, 0+), \\ \psi'(k, a-) &= K[\psi'(k, 0+) - \alpha\psi(k, 0)]. \end{aligned} \tag{2.6.29}$$

(a) *Define*

$$r(k) = \frac{\psi'(k, a/2+)}{\psi(k, a/2)}. \tag{2.6.30}$$

Then, as k^2 varies from the lower end of a gap in $\sigma(-\Delta_{\alpha,\Lambda})$ to the upper end, $r(k)$ is continuous with respect to k and strictly increasing in k^2. In particular, for $\alpha > 0$, $r(k)$ alternately increases from $-\infty$ to 0 or from 0 to $+\infty$ starting with $-\infty$ to 0 in the zeroth gap (i.e., the one starting at $-\infty$). For $\alpha < 0$, $r(k)$ increases from $-\infty$ to 0 in the zeroth gap and then alternately from $-\infty$ to 0 or from 0 to $+\infty$ starting with $-\infty$ to 0 in the first gap (cf. Figure 42).

(b) *Define*

$$\tilde{r}(k) = \frac{\psi'(k, 0+)}{\psi(k, 0+)} - (\alpha/2). \tag{2.6.31}$$

Then, as k^2 varies from the lower end of a gap in $\sigma(-\Delta_{\alpha,\Lambda})$ to the upper end, $\tilde{r}(k)$ is continuous with respect to k and strictly increasing in k^2. In particular, for $\alpha > 0$, $\tilde{r}(k)$ increases from $-\infty$ to 0 in all gaps (including the zeroth one), whereas for $\alpha < 0$, $\tilde{r}(k)$ increases from $-\infty$ to 0 in the zeroth gap and from 0 to $+\infty$ in all the remaining ones (cf. Figure 43).

PROOF. Inserting the ansatz

$$\psi(k, x) = \cos(kx) + A\sin(kx) \tag{2.6.32}$$

into (2.6.29) immediately yields for $k^2 \geq 0$

$$\begin{aligned} r(k) &= -\operatorname{sgn}(\xi(k))[k/2\sin(ka/2)][\xi(k)^2 - 1]^{1/2}\eta(k)^{-1}, \\ \tilde{r}(k) &= -\operatorname{sgn}(\xi(k))[k/\sin(ka)][\xi(k)^2 - 1]^{1/2}, \end{aligned} \tag{2.6.33}$$

where

$$\begin{aligned} \xi(k) &= \cos(ka) + (\alpha/2k)\sin(ka), \\ \eta(k) &= \cos(ka/2) + (\alpha/2k)\sin(ka/2), \qquad k^2 \geq 0. \end{aligned} \tag{2.6.34}$$

Similarly, for $k = i\kappa$, $\kappa > 0$, one infers

$$\begin{aligned} r(k) &= -\operatorname{sgn}(\xi(i\kappa))[\kappa/2\sinh(\kappa a/2)][\xi(i\kappa)^2 - 1]^{1/2}\eta(i\kappa)^{-1}, \\ \tilde{r}(k) &= -\operatorname{sgn}(\xi(i\kappa))[\kappa/\sinh(\kappa a)][\xi(i\kappa)^2 - 1]^{1/2}, \end{aligned} \tag{2.6.35}$$

where

$$\begin{aligned} \xi(i\kappa) &= \cosh(\kappa a) + (\alpha/2\kappa)\sinh(\kappa a), \\ \eta(i\kappa) &= \cosh(\kappa a/2) + (\alpha/2\kappa)\sinh(\kappa a/2), \qquad k = i\kappa, \quad \kappa > 0. \end{aligned} \tag{2.6.36}$$

Monotonicity of $r(k)$ and $\tilde{r}(k)$ now follows by checking dr/dk and $d\tilde{r}/dk$. The rest of the assertions concerning the range of r and $\tilde{r}$ in gaps follows from the explicit formulas above. ∎

We note that in part (a) of the above lemma the δ-interaction of strength α is placed in the center of the primitive cell as has been done in the definition of $-\Delta_{\alpha,\Lambda}(\theta)$ (cf. (2.3.13)). This case will be applied to interstitial impurities. On the other hand, part (b) describes a primitive cell shifted to the right by $a/2$ with respect to the one in part (a). Consequently, there are δ-interactions of strength $\alpha/2$ placed at $0+$ and $a-$. This case will be used for substitutional and defect impurities.

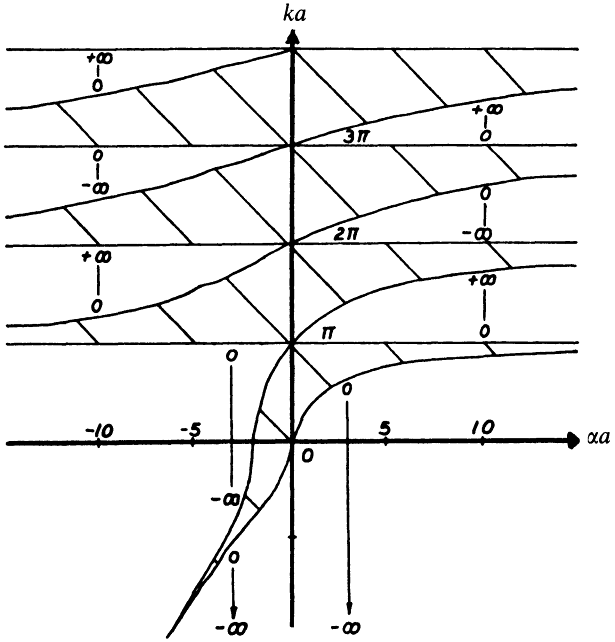


Figure 42 The range of r in the energy gaps. From Shrum and Peat, 1968, [411].

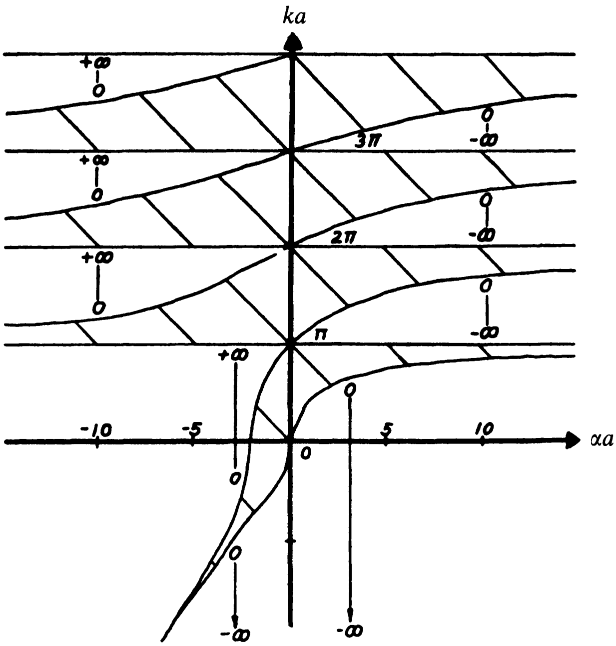


Figure 43 The range of $\tilde{r}$ in the energy gaps. From Shrum and Peat, 1968, [411].

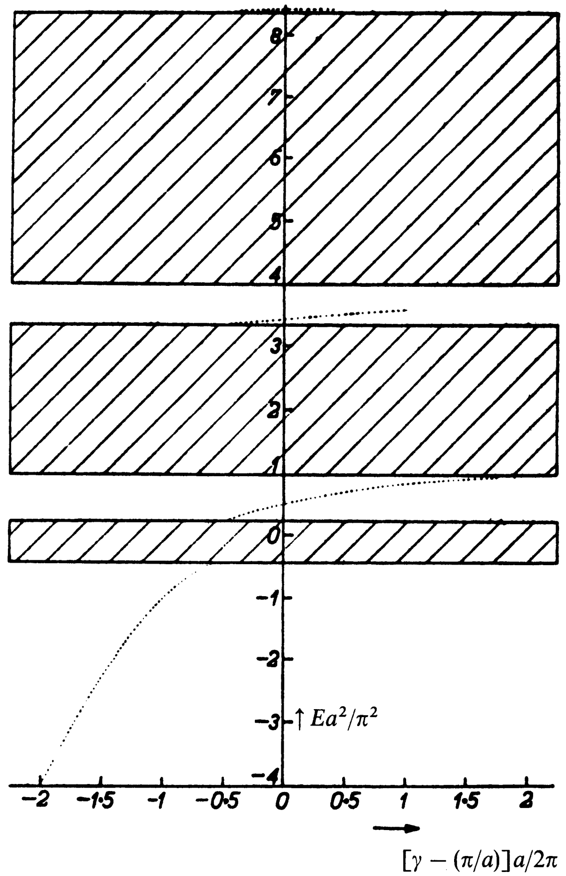


Figure 44 Cross-hatched regions denote the energy bands of $-\Delta_{-\pi/a,\Lambda,\gamma,z}$. Dotted lines indicate the extra energy levels due to a single substitutional impurity for varying impurity strength γ. From Saxon and Hutner, 1949, [404].

We have (cf. Figure 44).

Theorem 2.6.4. *Let the* substitutional δ-interaction *be concentrated at* $z \in \Lambda$ *with coupling constant* $\gamma \in \mathbb{R} - \{0\}$, $\gamma \neq -\alpha$. *Then the essential spectrum of* $-\Delta_{\alpha,\Lambda,\gamma,z}$ *is purely absolutely continuous and coincides with the band spectrum of* $-\Delta_{\alpha,\Lambda}$

$$\begin{aligned} \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,z}) &= \sigma_{\text{ac}}(-\Delta_{\alpha,\Lambda,\gamma,z}) = \sigma(-\Delta_{\alpha,\Lambda}), \\ \sigma_{\text{sc}}(-\Delta_{\alpha,\Lambda,\gamma,z}) &= \varnothing. \end{aligned} \tag{2.6.37}$$

(i) *For* $\alpha > 0$, $\gamma > 0$, $-\Delta_{\alpha,\Lambda,\gamma,z}$ *has no eigenvalues.*
(ii) *For* $\alpha > 0$, $\gamma < 0$, $-\Delta_{\alpha,\Lambda,\gamma,z}$ *has precisely one simple impurity state in every gap of its essential spectrum (including the zeroth one).*
(iii) *For* $\alpha < 0$, $\gamma > 0$ *there is precisely one simple impurity state in every gap except the zeroth one.*

(iv) *For $\alpha < 0, \gamma < 0$ there is precisely one simple eigenvalue below the first band and $-\Delta_{\alpha,\Lambda,\gamma,z}$ has no other eigenvalues.*

The equation for impurity states of energy $E = k^2$ of $-\Delta_{\alpha,\Lambda,\gamma,z}$ in $\mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,z})$ reads

$$\cot(ka) = (k/\alpha)[1 + (2k)^{-2}(\gamma^2 - \alpha^2)],$$
$$k^2 \in \mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,z}), \quad \operatorname{Im} k \geq 0, \quad (2.6.38)$$

with $\operatorname{Im} \theta(k) > 0$, $\operatorname{Re} \theta(k) \in (\pi/a)\mathbb{N}_0$, *where θ obeys the Kronig–Penney relation* (2.3.16).

Proof. The absence of embedded eigenvalues of $-\Delta_{\alpha,\Lambda,\gamma,z}$ in its essential spectrum follows from the condition $\operatorname{Im} \theta(k) > 0$ (cf. (2.6.21)) since only $\theta(k) \in \mathbb{R}$ gives rise to the band spectrum of $-\Delta_{\alpha,\Lambda}$. Relations (2.6.37) then follow from (2.6.10), (2.6.4), and Theorem XIII.20 in [391]. That there exists at most one simple impurity state in each gap is a consequence of Theorem 2.6.2 (or of the strict monotonicity of $\tilde{r}(k)$ in Lemma 2.6.3(b)). Observing $z = n_0 a$ for some $n_0 \in \mathbb{Z}$ and hence $z' = 0$, (2.6.27) simplifies to

$$-2ik \sin(\theta a) + \gamma \sin(ka) = 0, \qquad \operatorname{Im} k \geq 0, \quad \operatorname{Im} \theta > 0. \qquad (2.6.39)$$

Eliminating θ in (2.6.39) and in (2.3.16) yields (2.6.38). Clearly, $\operatorname{Re} \theta \in (\pi/a)\mathbb{N}_0$ to guarantee $k^2 \in \mathbb{R}$. The rest of the assertions now follow from Lemma 2.6.3(b) since the solutions $\Psi_{\alpha,\Lambda}(k, \pm 1, x)$ can only match at z to give there a δ-interaction of strength γ if $\tilde{r}(k) = \gamma/2$ (i.e., in particular, if their signs coincide) due to reflection symmetry of the bound state wave function near z. ∎

For the defect impurity we obtain (cf. Figure 45)

Theorem 2.6.5. *Let the* defect δ-interaction *be concentrated at $z \in \Lambda$ with coupling strength $-\alpha$. Then*

$$\begin{aligned} \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,-\alpha,z}) &= \sigma_{\text{ac}}(-\Delta_{\alpha,\Lambda,-\alpha,z}) = \sigma(-\Delta_{\alpha,\Lambda}), \\ \sigma_{\text{sc}}(-\Delta_{\alpha,\Lambda,-\alpha,z}) &= \varnothing. \end{aligned} \qquad (2.6.40)$$

(i) *For $\alpha > 0$, $-\Delta_{\alpha,\Lambda,-\alpha,z}$ has precisely one simple eigenvalue in all gaps of its essential spectrum (including the zeroth one).*
(ii) *For $\alpha < 0$, $-\Delta_{\alpha,\Lambda,-\alpha,z}$ has precisely one simple eigenvalue in all gaps of its essential spectrum except the zeroth one.*

The corresponding equation for defect levels $E = k^2$ of $-\Delta_{\alpha,\Lambda,-\alpha,z}$ in $\mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,-\alpha,z})$ reads

$$\cot(ka) = k/\alpha, \qquad k^2 \in \mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,-\alpha,z}), \quad \operatorname{Im} k \geq 0, \quad (2.6.41)$$

with $\operatorname{Im} \theta(k) > 0$, $\operatorname{Re} \theta(k) \in (\pi/a)\mathbb{N}_0$, *where θ solves* (2.3.16).

Proof. Taking $\gamma = -\alpha$ in (2.6.38) implies (2.6.41). The rest is analogous to the proof of Theorem 2.6.4 ∎

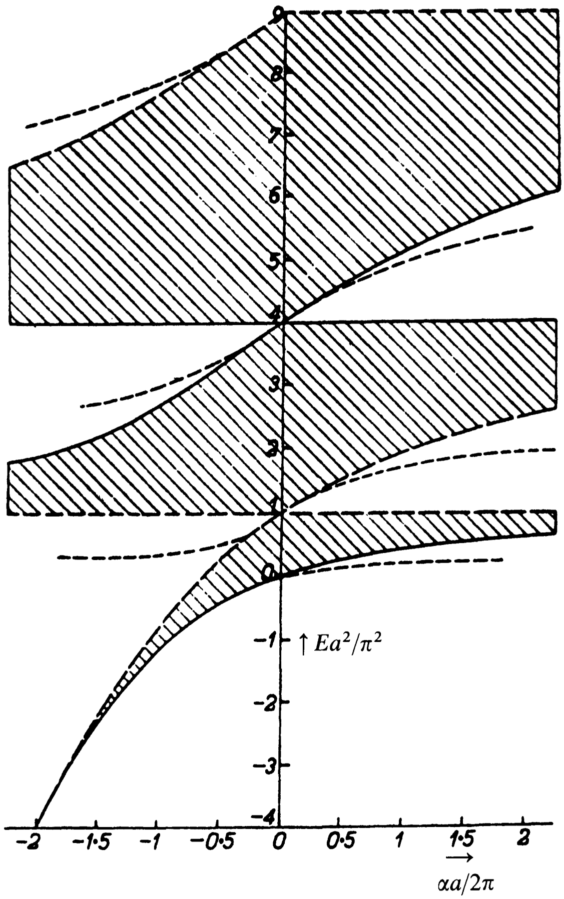


Figure 45 Cross-hatched regions denote the energy bands of $-\Delta_{\alpha,\Lambda,-\alpha,z}$ by varying α. Dashed lines show the extra energy levels due to a single defect point interaction of strength $-\alpha$. From Saxon and Hutner, 1949, [404].

Finally, we discuss an interstitial impurity (cf. Figure 46) in

Theorem 2.6.6. *Let the* interstitial δ-interaction *be placed at* $\tilde{z}$ *in the middle of two consecutive lattice points in* Λ *with a coupling constant* $\gamma \in \mathbb{R} - \{0\}$. *Then*

$$\begin{aligned} &\sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}) = \sigma_{\text{ac}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}) = \sigma(-\Delta_{\alpha,\Lambda}), \\ &\sigma_{\text{sc}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}) = \varnothing. \end{aligned} \tag{2.6.42}$$

(i) *For* $\alpha > 0, \gamma > 0$, $-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}$ *has a simple impurity level in every odd gap, whereas for* $\alpha > 0, \gamma < 0$ *there is a simple impurity level in all even gaps (including the zeroth one).*

(ii) *For* $\alpha < 0, \gamma > 0$ *there exists a simple impurity state in every even gap of* $\sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}})$ *except the zeroth one.*

(iii) *For* $\alpha < 0, \gamma < 0$ *there exists a simple bound state of* $-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}$ *in the zeroth gap and in all odd gaps of its essential spectrum.*

$-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}$ *has no other eigenvalues.*

The corresponding equation for impurity states $E = k^2$ of $-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}$ in $\mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}})$ reads

$$(\gamma/2k)^2 = \frac{(\alpha/2k)[\tan(ka/2)]^{-1} - 1}{(\alpha/2k)\tan(ka/2) + 1}, \quad k^2 \in \mathbb{R} - \sigma_{\text{ess}}(-\Delta_{\alpha,\Lambda,\gamma,\tilde{z}}), \quad \operatorname{Im} k \geq 0, \tag{2.6.43}$$

with $\operatorname{Im}\theta(k) > 0$, $\operatorname{Re}\theta(k) \in (\pi/a)\mathbb{N}_0$, where θ solves (2.3.16).

Proof. Since $\tilde{z} = (n_0 + \frac{1}{2})a$ for some $n_0 \in \mathbb{Z}$ we get $\tilde{z}' = a/2$ and thus (2.6.27) becomes

$$i\tan(\theta a/2) = (\gamma/2k)\tan(ka/2), \qquad \operatorname{Im} k \geq 0, \quad \operatorname{Im}\theta > 0. \tag{2.6.44}$$

Eliminating θ from (2.6.44) and (2.3.16) yields (2.6.43). The rest of the proof parallels that of Theorem 2.6.4 except that now Lemma 2.6.3(a) has to be applied in order to get solutions of $r(k) = \gamma/2$. ∎

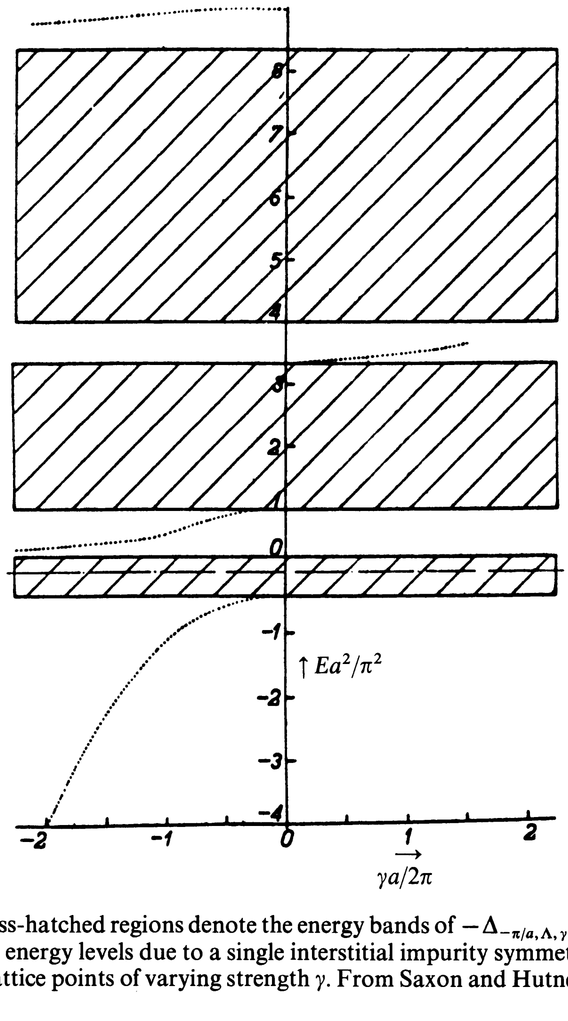


Figure 46 Cross-hatched regions denote the energy bands of $-\Delta_{-\pi/a,\Lambda,\gamma,\tilde{z}}$. Dotted lines show the extra energy levels due to a single interstitial impurity symmetrically located between two lattice points of varying strength γ. From Saxon and Hutner, 1949, [404].

Next we turn to impurity scattering. We are looking for scattering solutions $\Psi_{\alpha,\Lambda,\gamma,z}(k, \sigma, x)$ of $-\Delta_{\alpha,\Lambda,\gamma,z}$ fulfilling (2.6.18) and the boundary conditions (2.6.19) and (2.6.20) for $\sigma = +1$ and $\sigma = -1$ separately. Again for $x \in \mathbb{R} - \{z\}$ solutions $\psi(k)$ of $-\Delta_{\alpha,\Lambda,\gamma,z}\psi(k) = k^2\psi(k)$ also solve $-\Delta_{\alpha,\Lambda}\psi(k) = k^2\psi(k)$. Thus we are led to the ansatz

$$\Psi_{\alpha,\Lambda,\gamma,z}(k, +1, x) = \begin{cases} \mathscr{T}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k)\Psi_{\alpha,\Lambda}(k, +1, x), & x > z, \\ \Psi_{\alpha,\Lambda}(k, +1, x) + \mathscr{R}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k)\Psi_{\alpha,\Lambda}(k, -1, x), & x < z, \end{cases}$$

$$\Psi_{\alpha,\Lambda,\gamma,z}(k, -1, x) = \begin{cases} \Psi_{\alpha,\Lambda}(k, -1, x) + \mathscr{R}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k)\Psi_{\alpha,\Lambda}(k, +1, x), & x > z, \\ \mathscr{T}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k)\Psi_{\alpha,\Lambda}(k, -1, x), & x < z. \end{cases} \tag{2.6.45}$$

Insertion of (2.6.45) into (2.6.20) yields (suppressing α, Λ, γ, z in $\mathscr{T}^{\mathrm{l(r)}}_{\alpha,\Lambda,\gamma,z}(k)$ for a moment)

$$\begin{aligned} \mathscr{T}^{\mathrm{l}}(k)\Psi_{\alpha,\Lambda}(k, +1, z) &= \Psi_{\alpha,\Lambda}(k, +1, z) + \mathscr{R}^{\mathrm{l}}(k)\Psi_{\alpha,\Lambda}(k, -1, z), \\ \mathscr{T}^{\mathrm{r}}(k)\Psi_{\alpha,\Lambda}(k, -1, z) &= \Psi_{\alpha,\Lambda}(k, -1, z) + \mathscr{R}^{\mathrm{r}}(k)\Psi_{\alpha,\Lambda}(k, +1, z), \end{aligned} \tag{2.6.46}$$

and

$$\begin{aligned} &\mathscr{T}^{\mathrm{l}}(k)\Psi'_{\alpha,\Lambda}(k, +1, z+) - \Psi'_{\alpha,\Lambda}(k, +1, z-) - \mathscr{R}^{\mathrm{l}}(k)\Psi'_{\alpha,\Lambda}(k, -1, z-) \\ &\qquad = (\gamma + \alpha\delta_{z,\Lambda})\mathscr{T}^{\mathrm{l}}(k)\Psi_{\alpha,\Lambda}(k, +1, z), \\ &\Psi'_{\alpha,\Lambda}(k, -1, z+) + \mathscr{R}^{\mathrm{r}}(k)\Psi'_{\alpha,\Lambda}(k, +1, z+) - \mathscr{T}^{\mathrm{r}}(k)\Psi'_{\alpha,\Lambda}(k, -1, z-) \\ &\qquad = (\gamma + \alpha\delta_{z,\Lambda})\mathscr{T}^{\mathrm{r}}(k)\Psi_{\alpha,\Lambda}(k, -1, z). \end{aligned} \tag{2.6.47}$$

Employing again (2.6.24) we obtain

$$\begin{aligned} &[\mathscr{T}^{\mathrm{l}}(k) - 1]\Psi'_{\alpha,\Lambda}(k, +1, z+) - \mathscr{R}^{\mathrm{l}}(k)\Psi'(k, -1, z+) \\ &\qquad - \gamma\mathscr{T}^{\mathrm{l}}(k)\Psi_{\alpha,\Lambda}(k, +1, z) = 0, \\ &[1 - \mathscr{T}^{\mathrm{r}}(k)]\Psi'_{\alpha,\Lambda}(k, -1, z+) + \mathscr{R}^{\mathrm{r}}(k)\Psi'_{\alpha,\Lambda}(k, +1, z+) \\ &\qquad - \gamma\mathscr{T}^{\mathrm{r}}(k)\Psi_{\alpha,\Lambda}(k, -1, z) = 0. \end{aligned} \tag{2.6.48}$$

Solving (2.6.46) and (2.6.48) finally leads to

Theorem 2.6.7. *Let $\alpha, \gamma \in \mathbb{R} - \{0\}$, $z \in \mathbb{R}$. Then the unitary on-shell scattering matrix $\mathscr{S}_{\alpha,\Lambda,\gamma,z}(k)$ in $\mathbb{C}^2$ associated with the pair $(-\Delta_{\alpha,\Lambda,\gamma,z}, -\Delta_{\alpha,\Lambda})$ reads*

$$\mathscr{S}_{\alpha,\Lambda,\gamma,z}(k) = \begin{bmatrix} \mathscr{T}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k) & \mathscr{R}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k) \\ \mathscr{R}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k) & \mathscr{T}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k) \end{bmatrix}, \quad k^2 \in \sigma(-\Delta_{\alpha,\Lambda}), \ \operatorname{Im} k \geq 0, \tag{2.6.49}$$

where

$$\begin{aligned} \mathscr{T}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k) &= \frac{W(\overline{\Psi_{\alpha,\Lambda}(k, +1)}, \Psi_{\alpha,\Lambda}(k, -1))_{z+}}{W(\overline{\Psi_{\alpha,\Lambda}(k, +1)}, \Psi_{\alpha,\Lambda}(k, -1))_{z+} + \gamma\Psi_{\alpha,\Lambda}(k, +1, z)\Psi_{\alpha,\Lambda}(k, -1, z)} \\ &= \mathscr{T}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k), \end{aligned} \tag{2.6.50}$$

$$\mathscr{R}^{\mathrm{l}}_{\alpha,\Lambda,\gamma,z}(k) = \frac{-\gamma[\Psi_{\alpha,\Lambda}(k,+1,z)]^2}{W(\overline{\Psi_{\alpha,\Lambda}(k,+1)},\Psi_{\alpha,\Lambda}(k,-1))_{z+} + \gamma\Psi_{\alpha,\Lambda}(k,+1,z)\Psi_{\alpha,\Lambda}(k,-1,z)}, \tag{2.6.51}$$

$$\mathscr{R}^{\mathrm{r}}_{\alpha,\Lambda,\gamma,z}(k) = \frac{-\gamma[\Psi_{\alpha,\Lambda}(k,-1,z)]^2}{W(\overline{\Psi_{\alpha,\Lambda}(k,+1)},\Psi_{\alpha,\Lambda}(k,-1))_{z+} + \gamma\Psi_{\alpha,\Lambda}(k,+1,z)\Psi_{\alpha,\Lambda}(k,-1,z)}. \tag{2.6.52}$$

We emphasize that the vanishing of the denominator in (2.6.50)–(2.6.52) yields precisely the bound state condition (2.6.26). Using (2.6.27) and (2.6.11), the results (2.6.50)–(2.6.52) can be rewritten in terms of θ and k. We omit the details.

As $\gamma \to \infty$, the Dirichlet boundary condition at z implies

$$\mathscr{S}(k) = \begin{bmatrix} 0 & -\Psi_{\alpha,\Lambda}(k,-1,z)/\Psi_{\alpha,\Lambda}(k,+1,z) \\ -\Psi_{\alpha,\Lambda}(k,+1,z)/\Psi_{\alpha,\Lambda}(k,-1,z) & 0 \end{bmatrix}. \tag{2.6.53}$$

Obviously, the result of Theorems 2.6.4–2.6.6 and Theorem 2.6.7 can be derived using the finite difference approach described in Theorem 2.1.5. To illustrate this fact we consider the case of two half-crystals as in Sect. 2.4 with an impurity added at the beginning of one of the half-crystals. More precisely, let $-\Delta_{\alpha^{-+},\Lambda}$ describe the two half-crystals in (2.4.2) and add a δ-interaction of strength $\gamma \in \mathbb{R} - \{0\}$ at the origin (i.e., at the beginning of the right half-crystal). The resulting Hamiltonian in $L^2(\mathbb{R})$ is denoted by $-\Delta_{\alpha^{-+},\Lambda,\gamma}$. Then we obtain

Theorem 2.6.8. *Let the δ-type impurity be concentrated at zero with coupling constant $\gamma \in \mathbb{R} - \{0\}$. Then the essential spectrum of $-\Delta_{\alpha^{-+},\Lambda,\gamma}$ is purely absolutely continuous and coincides with the spectrum of $-\Delta_{\alpha^{-+},\Lambda}$*

$$\begin{aligned} &\sigma_{\mathrm{ess}}(-\Delta_{\alpha^{-+},\Lambda,\gamma}) = \sigma_{\mathrm{ac}}(-\Delta_{\alpha^{-+},\Lambda,\gamma}) = \sigma(-\Delta_{\alpha^{-+},\Lambda}), \\ &\sigma_{\mathrm{sc}}(-\Delta_{\alpha^{-+},\Lambda,\gamma}) = \varnothing. \end{aligned} \tag{2.6.54}$$

Moreover, there is at most one simple surface state in each gap of $\sigma_{\mathrm{ess}}(-\Delta_{\alpha^{-+},\Lambda,\gamma})$.

The corresponding bound state equation reads

$$\begin{aligned} &(-1)^{m_+}\{[(\alpha^+/2k)^2 - 1]\sin^2(ka) + (\alpha^+/k)\sin(ka)\cos(ka)\}^{1/2} \\ &\quad + (-1)^{m_-}\{[(\alpha^-/2k)^2 - 1]\sin^2(ka) + (\alpha^-/k)\sin(ka)\cos(ka)\}^{1/2} \\ &= [(\alpha^- - \alpha^+ - 2\gamma)/2k]\sin(ka), \quad \operatorname{Im} k \geq 0, \end{aligned} \tag{2.6.55}$$

where $\theta_\pm$ satisfy (*cf.* (2.4.25))

$$\begin{aligned} &\cos(\theta_\pm a) = \cos(ka) + (\alpha^\pm/2k)\sin(ka), \\ &\operatorname{Im}\theta_\pm > 0, \quad \operatorname{Re}\theta_\pm = m_\pm\pi/a, \quad m_\pm \in \mathbb{N}_0. \end{aligned} \tag{2.6.56}$$

PROOF. In order to obtain (2.6.55) we have to solve (suppressing the k-dependence for a moment)

$$\psi_{j+1} + \psi_{j-1} + \mu_j\psi_j = \varepsilon\psi_j, \qquad \psi_j \in \mathbb{C}, \quad j \in \mathbb{Z},$$

$$\varepsilon = 2\cos(ka), \qquad \mu_j = \begin{cases} \mu^+, & j = 1, 2, \ldots, \\ \mu_0, & j = 0, \\ \mu^-, & j = -1, -2, \ldots, \end{cases} \tag{2.6.57}$$

$$\mu^\pm = -\alpha^\pm k^{-1}\sin(ka), \qquad \mu_0 = -(\alpha^+ + \gamma)k^{-1}\sin(ka), \qquad k \neq m\pi/a, \quad m \in \mathbb{Z}.$$

For the surface state we make the ansatz

$$\psi_j = \begin{cases} c_+ e^{i\theta_+ aj}, & j = 0, 1, \ldots, \\ c_- e^{-i\theta_- aj}, & j = -1, -2, \ldots \end{cases} \qquad \mathrm{Im}\,\theta_\pm > 0, \quad \mathrm{Re}\,\theta_\pm \in (\pi/a)\mathbb{Z}. \tag{2.6.58}$$

Insertion of (2.6.58) into (2.6.57) yields

$$2\cos(\theta_+ a) = (\varepsilon - \mu^+) \qquad \text{for } j \geq 1, \tag{2.6.59}$$

$$\left.\begin{aligned} c_+ e^{i\theta_+ a} + c_- e^{i\theta_- a} &= (\varepsilon - \mu_0)c_+ \qquad \text{for } j = 0, \\ c_+ + c_- e^{2i\theta_- a} &= (\varepsilon - \mu^-)c_- e^{i\theta_- a} \qquad \text{for } j = -1, \end{aligned}\right. \tag{2.6.60}$$

$$2\cos(\theta_- a) = (\varepsilon - \mu^-) \qquad \text{for } j \leq -2. \tag{2.6.61}$$

Calculating the determinant associated with $c_\pm$ in (2.6.60) we get

$$[e^{2i\theta_- a} - (\varepsilon - \mu^-)e^{i\theta_- a}][e^{i\theta_+ a} - (\varepsilon - \mu_0)] - e^{i\theta_- a} = (\varepsilon - \mu_0) - e^{i\theta_- a} - e^{i\theta_+ a}. \tag{2.6.62}$$

Taking (2.6.62) equal to zero and eliminating $\theta_\pm$ with the help of (2.6.59) and (2.6.61) yields (2.6.55). Since necessarily $\mathrm{Im}\,\theta_\pm > 0$, to get an l^2-falloff as $j \to \pm\infty$ we infer from (2.4.6) that $-\Delta_{\alpha^{-+},\Lambda,\gamma}$ has no eigenvalues embedded in its essential spectrum. This together with Theorem 2.6.2 and the remark about the absolutely continuous spectrum in the proof of Theorem 2.4.1 yields the result. ■

In the "true" half-crystal situation where $\alpha^- = 0$, (2.6.55) simplifies to

$$\cot(ka) = -i[1 + 2(\gamma/\alpha^+)] + (\gamma/k)[1 + (\gamma/\alpha^+)]. \tag{2.6.63}$$

Generalizations placing the impurity in the interior of one of the half-crystals can now be obtained in an analogous manner (although quite tedious from a calculational point of view).

Notes

Section III.2.1

Self-adjointness of the operator $-\Delta_{\alpha,Y}$ defined in (2.1.6) follows, e.g., from [208], [345] (cf. also Appendix C). A numerical study of spectral concentration in the case where the points in $Y_{M,N}$ are equally spaced appeared in [397] (cf. Figure 40 in Sect. 2.3). The connection between $-\Delta_{\alpha,Y}$ in $L^2(\mathbb{R})$ and the discrete operator (2.1.49) goes back to Phariseau [373] (cf. also [400]) and Bellissard, Formoso, Lima, and Testard [70] (see also [478]). Our version of Theorem 2.1.5 is taken from [439].

Finite difference operators are discussed, e.g., in [46], [120], [122], [214].

The Kronig–Penney model on a Fibonacci lattice has been studied in [301].

Section III.2.2

Theorem 2.2.1 is taken from Albeverio, Gesztesy, Høegh-Krohn, and Kirsch [21]. Its proof is based on results of Morgan [345] and subsequent generalizations due to Kirsch [286] (cf. also Appendix C).

Section III.2.3

Direct integral decompositions and basic material in connection with periodic one-dimensional systems are treated in [54], [55], [160], [300], [326], [334], [391]. General periodic Schrödinger operators $H = -\Delta + V$ in $L^2(\mathbb{R}^d)$ are usually treated in p-space when $d \geq 2$, while x-space analysis is best adapted when $d = 1$, cf. [391], Sect. XIII.16.

Some generalizations of the Kronig–Penney model [307] (see also [185], [219], [449], [450], [486]) are studied, e.g., in [313], [384], [500], [501]. (For additional references in connection with surface states of half-crystals and random Kronig–Penney models we refer to the notes of the following sections.) The density of states (2.3.46) has been discussed in [215] using a different approach. (The sum (2.3.53) has been evaluated in [440].) The recursion scheme (2.3.64) and (2.3.65) appeared in [478]. A detailed treatment of mono- and diatomic lattices together with extensive illustrations can be found in [404]. In this paper the conjecture about the validity of Theorem 2.3.5 for binary alloys was also formulated. The proof of Theorem 2.3.5 in the special case of binary alloys actually appeared in [329] (cf. also [159]). That this result need not hold in general has been shown in [284] (cf. also [402]) using alloys consisting of certain square well interactions. The actual extension to general interactions taking into account the labeling of gaps involved appeared in [286]. Theorem 2.3.5 in the case of general alloys (consisting of equally spaced δ-interactions) is taken from [206] where a slightly different proof has been given. Theorem 2.3.6 is also taken from [206]. Other generalizations of Luttinger's theorem to general alloys of equally spaced δ-functions of definite sign of the coupling strengths (i.e., all $\gamma_n \geq 0$ or $\gamma_n \leq 0$, $n = 1, \ldots, N$) appeared in [286], [288], and [408]. Related, although not equivalent theorems on gaps in such alloys are treated in [254], [255], [256], [257], [259], [488], [489]. For the impossibility of the so-called inverse Saxon–Hutner conjecture, see, e.g., [166], [168], [169]. Lemma 2.3.8 is a standard result (see, e.g., [158], p. 1486).

In contrast to the three-dimensional treatment in Sect. III.1.4 we did not discuss the ε-expansion around the Kronig–Penney model. It is the purpose of the following to indicate how to fill in this gap. First of all, one easily computes that

$$\begin{aligned} g_k(\varepsilon x, \theta) &= \sum_{n\in\mathbb{Z}} G_k(\varepsilon x + an)e^{-i\theta an} \\ &= (i/2k)\{[1 - e^{i(k-\theta)a}]^{-1}e^{ik\varepsilon x} + [1 - e^{i(k+\theta)a}]^{-1}e^{-ik\varepsilon x} - e^{ik\varepsilon|x|}\} \\ &\underset{\varepsilon\downarrow 0}{=} \{\sin(ka)/2k[\cos(ka) - \cos(\theta a)]\} \\ &\quad - (\varepsilon/2)\{[1 - e^{i(k-\theta)a}]^{-1}x - [1 - e^{i(k+\theta)a}]^{-1}x + |x|\} + O(\varepsilon^2), \\ &\quad \varepsilon x \in (-a, a), \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k > 0, \quad \theta \in \bar{\hat{\Lambda}} = [-b/2, b/2]. \end{aligned}$$

Moreover, in analogy to (1.4.126)–(1.4.130) with $Y = \{0\}$ we introduce in $L^2(\mathbb{R})$

$$H_{\varepsilon,\Lambda} = -\Delta \dotplus \lambda(\varepsilon)\varepsilon^{-2} \sum_{\lambda\in\Lambda} V((\cdot - \lambda)/\varepsilon), \qquad \varepsilon > 0,$$

with $V \in L^1(\mathbb{R})$ being real-valued, supp(V) compact, and $\lambda(\varepsilon)$ analytic near $\varepsilon = 0$ with $\lambda(0) = 0$. Then obviously

$$\tilde{\mathscr{U}} H_{\varepsilon,\Lambda} \tilde{\mathscr{U}}^{-1} = \int_{[b/2,b/2)}^{\oplus} \frac{d\theta}{b} H_{\varepsilon,\Lambda}(\theta),$$

where (cf. (I.3.2.19))

$$\begin{aligned} (H_{\varepsilon,\Lambda}(-\theta) - k^2)^{-1} &= g_k(\theta) - \varepsilon^{-1}\lambda(\varepsilon)A_\varepsilon(k,\theta)[1 + B_\varepsilon(k,\theta)]^{-1}C_\varepsilon(k,\theta), \\ &\varepsilon > 0, \quad k^2 \in \rho(H_{\varepsilon,\Lambda}(-\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in [-b/2, b/2]. \end{aligned}$$

Here

$$\begin{aligned} &g_k(\theta)\colon L^2(\hat{\Gamma}) \to L^2(\hat{\Gamma}), \qquad g_k(\theta) = (-\Delta(-\theta) - k^2)^{-1}, \\ &A_\varepsilon(k,\theta)\colon L^2(\mathbb{R}) \to L^2(\hat{\Gamma}), \\ &B_\varepsilon(k,\theta)\colon L^2(\mathbb{R}) \to L^2(\mathbb{R}), \\ &C_\varepsilon(k,\theta)\colon L^2(\hat{\Gamma}) \to L^2(\mathbb{R}); \\ &\qquad \varepsilon \geq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in [-b/2, b/2] \end{aligned}$$

are operators with integral kernels

$$\begin{aligned} &g_k(v - v', \theta), \\ &A_\varepsilon(k, \theta, v, x) = g_k(v - \varepsilon x, \theta)v(x), \\ &B_\varepsilon(k, \theta, x, x') = \varepsilon^{-1}\lambda(\varepsilon)u(x)g_k(\varepsilon(x - x'), \theta)v(x'), \\ &C_\varepsilon(k, \theta, x, v) = u(x)g_k(\varepsilon x - v, \theta); \end{aligned}$$

$$\varepsilon \geq 0, \quad k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad x, x' \in \mathbb{R}, \quad v, v' \in \hat{\Gamma}, \quad \theta \in [-b/2, b/2].$$

Thus $B_\varepsilon(k, \theta)$ is analytic with respect to ε near $\varepsilon = 0$ in Hilbert–Schmidt norm. Consequently, one can follow the proof of Theorem I.3.3.1 in order to infer that for $\varepsilon > 0$ small enough and $\alpha = \lambda'(0)\int_{\mathbb{R}} dx\ V(x) \in \mathbb{R} - \{0\}$, all eigenvalues $E_{\varepsilon,\Lambda,m}(\theta)$, $m \in \mathbb{N}$, of $H_{\varepsilon,\Lambda}(\theta)$ are simple and analytic in ε near $\varepsilon = 0$

$$E_{\varepsilon,\Lambda,m}(\theta) = E_m^{\alpha,\Lambda}(\theta) + O(\varepsilon), \qquad \theta \in [-b/2, b/2), \quad m \in \mathbb{N}.$$

The first-order term in ε can be computed similarly to that in Theorem I.3.3.1.

The Stark effect in connection with the Kronig–Penney model is studied in [79], [352].

Section III.2.4

Scattering theory for general systems with different spatial asymptotics as $|x| \to \pm\infty$ has been considered in [118], [124], [136], [201], [401]. Spectral properties of one-dimensional half-crystals of δ-interactions are extensively treated in [3], [4], [5], [140], [212], [225], [304], [305], [340a], [343a], [356a], [372], [374], [376], [377], [422], [452], [453], [454], [458a], [458c], [460], [473], [474], [475], [478a], [487]. Theorem 2.4.2 appears to be new.

The Stark effect in connection with half-crystals of δ-interactions is studied in [58], [73], [76], [77], [455], [458], [458b].

Section III.2.5

The idea of exploiting the condition between $h(\lambda, \theta, \phi)$ and $-\Delta_{y(\theta,\phi),\Lambda}$ in the quasi-periodic case is due to Bellissard, Formoso, Lima, and Testard [70]. Theorem 2.5.1(a) has been suggested by Aubry [48] and was proven by Avron and Simon [56]. Theorem 2.5.1(b) is also due to [56] (cf. also [439]). Theorem 2.5.1(c), (d) is taken from Bellissard, Lima, and Testard [71]. For discussions in the physics literature, cf. [48], [49], [57], [238], [246], [263], [447], and [448].

Section III.2.6

Theorem 2.6.1 in the context of three-dimensional point interactions appeared in Albeverio, Høegh-Krohn, and Mebkhout [31]. Depending on the decay properties of $G_{k,\alpha,Y}(x, z_l)$, $k^2 \in \rho(-\Delta_{\alpha,Y})$, $\operatorname{Im} k > 0$, as $|x| \to \infty$, formula (2.6.4) extends to infinitely many impurities in a discrete set Z with $|z_l - z_{l'}| \geq d > 0$ for all $z_l \neq z_{l'}$, z_l, $z_{l'} \in Z$, along the lines of Theorem 2.1.3.

The number of impurity levels in gaps of the essential spectrum is discussed in [137], [258], [296], [404], [411], [423], and [459].

Tunneling phenomena are treated in [409], [410], and [461].

The Kronig–Penney Bloch wave functions (2.6.11) and their derivation has been taken from Saxon and Hutner [404]. In this paper the corresponding Bloch wave function of a diatomic lattice (i.e., the sequence α is periodic with period two, $\alpha_{j+2} = \alpha_j$, $j \in \mathbb{Z}$, $\alpha_0 = \alpha$, $\alpha_1 = \beta$, $\alpha \neq \beta$, α, $\beta \in \mathbb{R}$) is also given. Lemma 2.6.3 is taken from Schrum and Peat [411]. The results of Theorems 2.6.4–2.6.6 together with numerical illustrations can be found in [404] and [411]. See also [281a] for a discussion on impurity levels. Substitutional impurities in a diatomic lattice are also discussed in [404]. We note that δ'-type interstitial impurities can be treated in analogy to Theorem 2.6.6.

The explicit results on impurity scattering in the Kronig–Penney model in Theorem 2.6.7 appear to be new. Again an interstitial δ-interaction could be replaced by an interstitial δ'-interaction. The result (2.6.54) (for $\alpha^- = 0$) and other generalizations together with numerical illustrations are contained in papers by Aerts [3], [4], [5].

CHAPTER III.3

Infinitely Many δ'-Interactions in One Dimension

Now we derive the main results of Ch. 2 for δ'- instead of δ-interactions. We shall closely follow the strategy for δ-interactions and only present detailed proofs if the arguments differ substantially from those in Ch. 2.

Let $J \subset \mathbb{Z}$ be the index set of Sect. 2.1 and $Y = \{y_j \in \mathbb{R} \mid j \in J\}$ be a discrete subset of $\mathbb{R}$ satisfying (2.1.1) and the remarks after (2.1.1). In analogy to Ch. II.3 we introduce the minimal operator $\dot{H}'_Y$ in $L^2(\mathbb{R})$

$$\dot{H}'_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\dot{H}'_Y) = \{g \in H^{2,2}(\mathbb{R}) \mid g'(y_j) = 0,\ y_j \in Y, j \in J\}. \quad (3.1)$$

Then $\dot{H}'_Y$ is closed and nonnegative and its adjoint operator reads

$$\begin{aligned} \dot{H}'^{*}_Y &= -\frac{d^2}{dx^2}, \\ \mathscr{D}(\dot{H}'^{*}_Y) &= \{g \in H^{2,2}(\mathbb{R} - Y) \mid g'(y_j+) = g'(y_j-),\ y_j \in Y, j \in J\}. \end{aligned} \quad (3.2)$$

The equation

$$\dot{H}'^{*}_Y \phi(k) = k^2 \phi(k), \qquad \phi(k) \in \mathscr{D}(\dot{H}'^{*}_Y), \quad k^2 \in \mathbb{C} - \mathbb{R}, \quad \operatorname{Im} k > 0, \quad (3.3)$$

then has the solutions

$$\phi_j(k, x) = \begin{cases} e^{ik(x-y_j)}, & x > y_j, \\ -e^{ik(y_j-x)}, & x < y_j, \end{cases} \qquad \operatorname{Im} k > 0, \quad y_j \in Y, \quad j \in J, \quad (3.4)$$

which span the deficiency subspace of $\dot{H}'_Y$. Thus $\dot{H}'_Y$ has deficiency indices (∞, ∞). According to Appendix C a particular type of self-adjoint extensions of $\dot{H}'_Y$ is of the type

$$\Xi_{\beta,Y} = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\Xi_{\beta,Y}) = \{g \in H^{2,2}(\mathbb{R} - Y) | g'(y_j+) = g'(y_j-),$$
$$g(y_j+) - g(y_j-) = \beta_j g'(y_j), j \in J\},$$
$$\beta = \{\beta_j\}_{j \in J}, \quad -\infty < \beta_j \le \infty, \quad j \in J. \quad (3.5)$$

By definition $\Xi_{\beta,Y}$ describes δ'-interactions of strength β_j centered at $y_j \in Y$, $j \in J$. The special case $\beta_j = 0, j \in J$, leads to the kinetic energy operator $-\Delta$ on $H^{2,2}(\mathbb{R})$ whereas the case $\beta_{j_0} = \infty$ for some $j_0 \in J$ leads to a Neumann boundary condition at the point y_{j_0} (i.e., $g'(y_{j_0}+) = g'(y_{j_0}-) = 0$).

Since Theorems 2.1.1 and 2.1.2 immediately go through with $-\Delta_{\alpha,Y}$, $-\Delta_{\alpha_{M,N},Y_{M,N}}$ replaced by their respective analogs, we directly proceed to a description of the resolvent of $\Xi_{\beta,Y}$.

Theorem 3.1. *Let $\beta_j \in \mathbb{R} - \{0\}, j \in J$, and assume* (2.1.1). *Then*

$$(\Xi_{\beta,Y} - k^2)^{-1} = G_k + \sum_{j,j' \in J} [\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} (\overline{\tilde{\tilde{G}}_k(\cdot - y_{j'})}, \cdot) \tilde{\tilde{G}}_k(\cdot - y_j),$$
$$k^2 \in \rho(\Xi_{\beta,Y}), \quad \operatorname{Im} k > 0. \quad (3.6)$$

Here

$$\tilde{\Gamma}_{\beta,Y}(k) = [-(\beta_j k^2)^{-1} \delta_{jj'} + G_k(y_j - y_{j'})]_{j,j' \in J}, \qquad \operatorname{Im} k > 0, \quad (3.7)$$

is a closed operator in $l^2(Y)$ with

$$[\tilde{\Gamma}_{\beta,Y}(k)]^{-1} \in \mathscr{B}(l^2(Y)), \qquad k^2 \in \rho(\Xi_{\beta,Y}), \quad \operatorname{Im} k > 0 \quad \text{large enough}, \quad (3.8)$$

and

$$\begin{aligned} \tilde{\tilde{G}}_k(x - y) &= (i/2k) \begin{cases} e^{ik(x-y)}, & x > y, \\ -e^{ik(y-x)}, & x < y, \end{cases} \\ G_k(x - y) &= (i/2k) e^{ik|x-y|}, \quad \operatorname{Im} k > 0. \end{aligned} \quad (3.9)$$

PROOF. One can follow the proof of Theorem 2.1.3 step by step since obviously $|\tilde{\tilde{G}}_k(x)| = |G_k(x)|$. ■

The analog of Theorem 2.1.4 then reads

Theorem 3.2. *Let $\beta_j \in \mathbb{R} - \{0\}, j \in J$, and assume* (2.1.1). *Then the domain $\mathscr{D}(\Xi_{\beta,Y})$ consists of all elements ψ of the type*

$$\psi(x) = \phi_k(x) + (i/k) \sum_{j,j' \in J} [\tilde{\Gamma}_{\beta,Y}(k)]^{-1}_{jj'} \phi'_k(y_{j'}) \tilde{\tilde{G}}_k(x - y_j), \quad (3.10)$$

where $\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R})$ and $k^2 \in \rho(\Xi_{\beta,Y})$, $\operatorname{Im} k > 0$. The decomposition (3.10) *is unique and with $\psi \in \mathscr{D}(\Xi_{\beta,Y})$ of this form we obtain*

$$(\Xi_{\beta,Y} - k^2)\psi = (-\Delta - k^2)\phi_k. \quad (3.11)$$

Next let $\psi \in \mathscr{D}(\Xi_{\beta,Y})$ and suppose that $\psi = 0$ in an open set $U \subseteq \mathbb{R}$. Then $\Xi_{\beta,Y}\psi = 0$ in U.

Having established some of the basic properties of $\Xi_{\beta,Y}$ we now turn to a one-to-one correspondence between $\Xi_{\beta,Y}$ and a certain discrete operator in $l^2(Y)$. Actually, it will turn out that this discrete operator is almost identical to the one we discussed in connection with $-\Delta_{\alpha,Y}$ at the end of Sect. 2.1. Our strategy now will be somewhat different to that in Sect. 2.1 since we shall directly derive the corresponding difference equation without intermediate matrix transformations. As in Sect. 2.1 we assume without loss of generality $J = \mathbb{Z}$ and suppose $\pm\infty$ to be the only accumulation points of Y such that $\mathbb{R} = \bigcup_{j\in\mathbb{Z}} I_j$. We intend to solve

$$(\Xi_{\beta,Y} - k^2)\psi(k, x) = 0, \qquad \operatorname{Im} k \geq 0, \quad x \in \mathbb{R} - Y, \tag{3.12}$$

with boundary conditions

$$\psi'(k, y_j+) = \psi'(k, y_j-), \quad \psi(k, y_j+) - \psi(k, y_j-) = \beta_j\psi'(k, y_j), \quad \beta_j \in \mathbb{R},\ j \in \mathbb{Z}. \tag{3.13}$$

On every interval $\mathring{I}_{j+1}$ we obtain

$$\begin{aligned}
\psi(k, x) &= \psi(k, y_j+)\cos[k(x - y_j)] + \psi'(k, y_j)k^{-1}\sin[k(x - y_j)],\\
\psi'(k, x) &= -\psi(k, y_j+)k\sin[k(x - y_j)] + \psi'(k, y_j)\cos[k(x - y_j)],\\
&\qquad \operatorname{Im} k \geq 0, \quad x \in \mathring{I}_{j+1}.
\end{aligned} \tag{3.14}$$

Thus we infer

$$\begin{aligned}
\psi'(k, y_{j+1}) &= -\psi(k, y_j+)k\sin[k(y_{j+1} - y_j)] + \psi'(k, y_j)\cos[k(y_{j+1} - y_j)],\\
\psi'(k, y_j) &= -\psi(k, y_{j-1}+)k\sin[k(y_j - y_{j-1})]\\
&\quad + \psi'(k, y_{j-1})\cos[k(y_j - y_{j-1})],\\
\psi(k, y_j-) &= \psi(k, y_{j-1}+)\cos[k(y_j - y_{j-1})] + \psi'(k, y_{j-1})k^{-1}\sin[k(y_j - y_{j-1})].
\end{aligned} \tag{3.15}$$

Using (3.15), a simple calculation then yields

$$\begin{aligned}
\psi'(k, y_{j+1}) &= -[\psi(k, y_j-) + \beta_j\psi'(k, y_j)]k\sin[k(y_{j+1} - y_j)]\\
&\quad + \psi'(k, y_j)\cos[k(y_{j+1} - y_j)]\\
&= \left\{-\beta_j k\sin[k(y_{j+1} - y_j)] + \frac{\sin[k(y_{j+1} - y_{j-1})]}{\sin[k(y_j - y_{j-1})]}\right\}\psi'(k, y_j)\\
&\quad - \psi'(y_{j-1})\frac{\sin[k(y_{j+1} - y_j)]}{\sin[k(y_j - y_{j-1})]},\\
&\qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z},
\end{aligned} \tag{3.16}$$

or equivalently,

$$\begin{aligned}
&\sin[k(y_j - y_{j-1})]\psi_{j+1}(k) + \sin[k(y_{j+1} - y_j)]\psi_{j-1}(k)\\
&\quad = \{-\beta_j k\sin[k(y_{j+1} - y_j)]\sin[k(y_j - y_{j-1})] + \sin[k(y_{j+1} - y_{j-1})]\}\psi_j(k),\\
&\qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z},
\end{aligned} \tag{3.17}$$

$$\psi_j(k) \equiv \psi'(k, y_j), \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}.$$

We emphasize the great similarity of (3.17) and (2.1.49): The only difference concerns the term α_j/k which goes into $-\beta_j k$. Defining

$$\Phi_j(k) = \begin{bmatrix} \psi'(k, y_j) \\ \psi'(k, y_{j-1}) \end{bmatrix} \equiv \begin{bmatrix} \psi_j(k) \\ \psi_{j-1}(k) \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{3.18}$$

and

$$M_j(k) = \begin{bmatrix} -\beta_j k \sin[k(y_{j+1} - y_j)] + \dfrac{\sin[k(y_{j+1} - y_{j-1})]}{\sin[k(y_j - y_{j-1})]} & -\dfrac{\sin[k(y_{j+1} - y_j)]}{\sin[k(y_j - y_{j-1})]} \\ 1 & 0 \end{bmatrix},$$

$$\operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \tag{3.19}$$

then (3.17) can be rewritten in matrix form

$$M_j(k)\Phi_j(k) = \Phi_{j+1}(k), \qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}. \tag{3.20}$$

Moreover, we get

Theorem 3.3. *Let $\beta_j \in \mathbb{R}, j \in \mathbb{Z}$. Then any solution $\psi(k, x)$, $k^2 \in \mathbb{R}$, $\operatorname{Im} k \geq 0$, $k \neq \pi m(y_j - y_{j-1})^{-1}, j, m \in \mathbb{Z}$, of* (3.12) *and* (3.13) *satisfies* (3.17). *Conversely, any solution of* (3.17) *defines via*

$$\psi(k, x) = \psi_j(k)k^{-1} \sin[k(x - y_j)] + \{-\psi_{j+1}(k) + \psi_j(k) \cos[k(y_{j+1} - y_j)]\} \frac{\cos[k(x - y_j)]}{k \sin[k(y_{j+1} - y_j)]},$$

$$x \in \mathring{I}_{j+1}, \quad k^2 \in \mathbb{R}, \quad \operatorname{Im} k \geq 0, \quad k \neq \pi m(y_j - y_{j-1})^{-1}, \quad j, m \in \mathbb{Z}, \tag{3.21}$$

a solution of (3.12) *and* (3.13). *In addition, $\psi(k) \in L^p(\mathbb{R})$ implies $\{\psi_j(k) = \psi'(k, y_j)\}_{j \in \mathbb{Z}} \in l^p(\mathbb{Z})$ for $p = \infty$ or $p = 2$. Moreover, exponential growth (resp. decay) of $\psi(k, x)$ implies that of $\{\psi_j(k)\}_{j \in \mathbb{Z}}$ and at the same rate (cf. Theorem* 2.1.5). *In the special case of a lattice structure of Y, i.e., $y_{j+1} - y_j = a > 0, j \in \mathbb{Z}$, the last two statements may be reversed, i.e., $\{\psi_j(k) = \psi'(k, y_j)\}_{j \in \mathbb{Z}} \in l^p(\mathbb{Z})$ implies $\psi(k) \in L^p(\mathbb{R})$ for $p = \infty$ or $p = 2$, and similarly for the exponential growth rate.*

PROOF. Using (2.1.51)–(2.1.53) and

$$\begin{aligned} &\psi'(k, y_j) = \psi'(k, x) \cos[k(x - y_j)] + \psi(k, x)k \sin[k(x - y_j)], \qquad x \in \mathring{I}_{j+1}, \\ &[\psi(k, x)]^2 + k^{-2}[\psi'(k, x)]^2 = k^{-2}[\psi_j(k)]^2 \\ &+ k^{-2} \sin^{-2}[k(y_{j+1} - y_j)]\{-\psi_{j+1}(k) + \psi_j(k) \cos[k(y_{j+1} - y_j)]\}^2, \qquad x \in \mathring{I}_{j+1}, \end{aligned} \tag{3.22}$$

(taking ψ real-valued) one can follow the corresponding proof of Theorem 2.1.5 step by step. ∎

Next, we consider a periodic lattice and assume $Y = \Lambda \equiv a\mathbb{Z}$, $a > 0$. In this case $M_j(k)$ simplifies to

$$M_j(k) = \begin{bmatrix} -\beta_j k \sin(ka) + 2\cos(ka) & -1 \\ 1 & 0 \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \quad (3.23)$$

and (3.17) becomes

$$\psi_{j+1}(k) + \psi_{j-1}(k) = \{-\beta_j k \sin(ka) + 2\cos(ka)\}\psi_j(k),$$
$$\operatorname{Im} k \geq 0, \quad k \neq \pi m/a, \quad j, m \in \mathbb{Z}. \quad (3.24)$$

Of course, the remarks after (2.1.55) apply as well in the present case. As our first concrete example we discuss the analog of the Kronig–Penney model for δ'-interactions. The corresponding Hamiltonian in $L^2(\mathbb{R})$ reads

$$\Xi_{\beta,\Lambda} = -\frac{d^2}{dx^2},$$
$$\mathscr{D}(\Xi_{\beta,\Lambda}) = \{g \in H^{2,2}(\mathbb{R} - \Lambda) | g'(na+) = g'(na-),$$
$$g(na+) - g(na-) = \beta g'(na), n \in \mathbb{Z}\},$$
$$-\infty < \beta \leq \infty \quad (3.25)$$

and we adopt the notation of Sect. 2.3. In analogy to (2.3.13) we also introduce in $L^2((-a/2, a/2))$ the family of self-adjoint operators

$$\Xi_{\beta,\Lambda}(\theta) = -\frac{d^2}{dv^2},$$
$$\mathscr{D}(\Xi_{\beta,\Lambda}(\theta)) = \{g(\theta) \in H^{2,2}((-a/2, a/2) - \{0\}) | g(\theta, -a/2+) = e^{i\theta a} g(\theta, a/2-),$$
$$g'(\theta, -a/2+) = e^{i\theta a} g'(\theta, a/2-),$$
$$g'(\theta, 0+) = g'(\theta, 0-), g(\theta, 0+) - g(\theta, 0-) = \beta g'(\theta, 0)\},$$
$$-\infty < \beta \leq \infty, \quad \theta \in [-b/2, b/2). \quad (3.26)$$

Then we have

Theorem 3.4. *Let $-\infty < \beta \leq \infty$, $\theta \in [-b/2, b/2)$. Then the essential spectrum of $\Xi_{\beta,\Lambda}(\theta)$ is empty,*

$$\sigma_{\text{ess}}(\Xi_{\beta,\Lambda}(\theta)) = \phi \quad (3.27)$$

and thus the spectrum of $\Xi_{\beta,\Lambda}(\theta)$ is purely discrete. In particular, its eigenvalues $E_m^{\beta,\Lambda}(\theta)$, $m \in \mathbb{N}$, ordered in magnitude are given by

$$E_m^{\beta,\Lambda}(\theta) = [k_m^{\beta,\Lambda}(\theta)]^2, \qquad m \in \mathbb{N}, \quad (3.28)$$

where $k_m^{\beta,\Lambda}(\theta)$, $m \in \mathbb{N}$, are solutions of

$$\cos(\theta a) = \cos(ka) - (\beta k/2)\sin(ka), \qquad \operatorname{Im} k \geq 0. \quad (3.29)$$

For $\beta \in \mathbb{R} - \{0\}$, except for $\beta = -a$, $m = 1$, and $\theta = 0$, the eigenvalues

$E_m^{\beta,\Lambda}(\theta)$ are simple with corresponding eigenfunctions

$$g_m^{\beta,\Lambda}(\theta, v) = C \begin{cases} e^{ik_m^{\beta,\Lambda}(\theta)v} + e^{i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a}\dfrac{1 - e^{-i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a}}{e^{i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a} - 1}e^{-ik_m^{\beta,\Lambda}(\theta)v}, \\ \qquad\qquad -a/2 < v < 0, \\ e^{-i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a}e^{ik_m^{\beta,\Lambda}(\theta)v} + \dfrac{1 - e^{-i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a}}{e^{i\theta a}e^{-ik_m^{\beta,\Lambda}(\theta)a} - 1}e^{-ik_m^{\beta,\Lambda}(\theta)v}, \\ \qquad\qquad 0 < v < a/2, \\ m \in \mathbb{N}, \quad \theta \in [-b/2, b/2) \text{ and } m \geq 2 \text{ for } \beta = -a \text{ and } \theta = 0. \end{cases} \tag{3.30}$$

If $\beta = -a$, then $E_1^{-a,\Lambda}(0) = 0$ is a twice degenerate eigenvalue with corresponding eigenfunctions

$$g_{1,1}^{-a,\Lambda}(0, v) = 1, \qquad g_{1,2}^{-a,\Lambda}(0, v) = \begin{cases} 1 + v, & -a/2 < v < 0, \\ 1 - a + v, & 0 < v < a/2. \end{cases} \tag{3.31}$$

We have

$$\begin{aligned} E_1^{\beta,\Lambda}(0) &= 0 < E_1^{\beta,\Lambda}(-b/2) < E_2^{\beta,\Lambda}(-b/2) = \pi^2/a^2 < E_2^{\beta,\Lambda}(0) < E_3^{\beta,\Lambda}(0) \\ &= 4\pi^2/a^2 < E_3^{\beta,\Lambda}(-b/2) < E_4^{\beta,\Lambda}(-b/2) = 9\pi^2/a^2 \\ &< E_4^{\beta,\Lambda}(0) < E_5^{\beta,\Lambda}(0) = 16\pi^2/a^2 \\ &< E_5^{\beta,\Lambda}(-b/2) < \cdots, \qquad \beta > 0, \end{aligned} \tag{3.32}$$

$$\begin{aligned} E_1^{\beta,\Lambda}(-b/2) &< E_1^{\beta,\Lambda}(0) < E_2^{\beta,\Lambda}(0) < E_2^{\beta,\Lambda}(-b/2) = \pi^2/a^2 \\ &< E_3^{\beta,\Lambda}(-b/2) < E_3^{\beta,\Lambda}(0) = 4\pi^2/a^2 \\ &< E_4^{\beta,\Lambda}(0) < E_4^{\beta,\Lambda}(-b/2) = 9\pi^2/a^2 \\ &< E_5^{\beta,\Lambda}(-b/2) < \cdots, \end{aligned}$$

$$E_1^{\beta,\Lambda}(-b/2) < 0,$$

$$E_1^{\beta,\Lambda}(0) \begin{cases} <0, & |\beta| < a, \\ =0, & |\beta| \geq a, \end{cases} \qquad E_2^{\beta,\Lambda}(0) \begin{cases} =0, & |\beta| \leq a, \\ >0, & |\beta| > a, \end{cases} \qquad \beta < 0. \tag{3.33}$$

All nonconstant eigenvalues $E_m^{\beta,\Lambda}(\theta)$, $\theta \in [-b/2, b/2)$, $m \in \mathbb{N}$, are strictly decreasing with respect to $\beta \in \mathbb{R}$.

For $\beta = 0$ the eigenvalues and eigenfunctions are identical to those given in (2.3.20). For $\beta = \infty$ the Neumann boundary condition at zero implies simple eigenvalues $E_m^{\infty,\Lambda}$ for $m \geq 2$ and a twice degenerate ground state $E_1^{\infty,\Lambda}$

$$E_1^{\infty,\Lambda} = 0,$$

$$g_{1,1}^{\infty,\Lambda}(v) = \begin{cases} 1, & -a/2 < v < 0, \\ 0, & 0 < v < a/2, \end{cases} \qquad g_{1,2}^{\infty,\Lambda}(v) = \begin{cases} 0, & -a/2 < v < 0, \\ 1, & 0 < v < a/2, \end{cases}$$

$$E_m^{\infty,\Lambda} = (m-1)^2\pi^2/a^2,$$

$$g_m^{\infty,\Lambda}(\theta, v) = C\cos((m-1)\pi v/a)\begin{cases}1, & -a/2 < v < 0\\ (-1)^{m-1}e^{-i\theta a}, & 0 < v < a/2,\end{cases}$$

$$m = 2, 3, \ldots. \quad (3.34)$$

PROOF. Since $\Xi_{\beta,\Lambda}(\theta)$ obviously has compact resolvent we infer (3.27). Since the results (3.30), (3.31), and (3.34) follow again from straightforward computations we concentrate on (3.29), (3.32), and (3.33). Nondegeneracy of the eigenvalues $E_m^{\beta,\Lambda}(\theta)$ for $\theta \in (-b/2, 0) \cup (0, b/2)$ follows as in the proof of Theorem 2.3.1. In order to derive (3.29) one can either use an approach based on (3.26) or our difference equation approach. Since the latter works more quickly we use the ansatz

$$\psi_j(k) = e^{\pm i\theta(k)aj}, \qquad \operatorname{Im}\theta(k) \geq 0, \quad j \in \mathbb{Z}, \tag{3.35}$$

in (3.24) and (3.29) immediately results. As in the proof of Theorem 2.3.1 we now concentrate on the cases $\theta = 0, -b/2$. Thus we look for solutions of

$$\begin{aligned} \pm 1 &= \cos(ka) - (\beta k/2)\sin(ka), && k \geq 0,\\ \pm 1 &= \cosh(\kappa a) + (\beta\kappa/2)\sinh(\kappa a), && k = i\kappa, \quad \kappa \geq 0. \end{aligned} \tag{3.36}$$

This in turn is equivalent to solving

$$\sin(ka/2) = 0 \quad \text{or} \quad \cot(ka/2) = -2/\beta k \qquad \text{for} \quad \theta = 0, \tag{3.37}$$

$$\sin[(ka+\pi)/2] = 0 \quad \text{or} \quad \cot[(ka+\pi)/2] = -2/\beta k \qquad \text{for} \quad \theta = -b/2; \quad k \geq 0, \tag{3.38}$$

and for nonpositive energies to

$$\sinh(\kappa a/2) = 0 \quad \text{or} \quad 1 = (-\beta\kappa/2)\coth(\kappa a/2) \qquad \text{for} \quad \theta = 0, \tag{3.39}$$

$$1 = (-\beta\kappa/2)\tanh(\kappa a/2) \qquad \text{for} \quad \theta = -b/2; \quad k = i\kappa, \quad \kappa > 0. \tag{3.40}$$

We study the case with nonpositive energy first. Obviously, (3.39) and (3.40) have no solutions for $\beta \geq 0$ except $\kappa = 0$. For $\beta < 0$ we use

$$\begin{aligned} &x\coth(x) \geq 1, && x\coth(x) \geq x,\\ &x\tanh(x) \leq x, && x\tanh(x) \leq x\coth(x), \qquad x \geq 0, \end{aligned} \tag{3.41}$$

to infer that (cf. Figure 47(a)) (3.40) has precisely one solution $\kappa_1(\beta) > 0$, $\beta < 0$, and (3.39) has as only solutions

$$\begin{aligned} &\kappa_2(\beta) = 0, \qquad 0 < \kappa_3(\beta) < \kappa_1(\beta) \qquad \text{for} \quad 0 < |\beta| < a,\\ &\kappa_2(\beta) = 0 \qquad \text{for} \quad |\beta| \geq a. \end{aligned} \tag{3.42}$$

(If $\beta = -a$ then both equations in (3.39) yield precisely zero as solutions.) Next we turn to nonnegative energies. We start with the simpler case $\beta > 0$. Then (3.37) and (3.38) yield solutions $k_n = n\pi/a$, $n \in \mathbb{N}_0$, and, since $\cot(ka/2)$ is strictly decreasing from $+\infty$ to $-\infty$ in $(2n\pi/a, 2(n+1)\pi/a)$, $n \in \mathbb{N}_0$, and $\cot[(ka+\pi)/2]$ is strictly decreasing from 0 to $-\infty$ in $(0, \pi/a)$ and from $+\infty$ to $-\infty$ in $((2n+1)\pi/a, (2n+3)\pi/a)$, $n \in \mathbb{N}_0$, one has precisely one additional solution in every interval $(n\pi/a, (n+1)\pi/a)$, $n \in \mathbb{N}_0$ (cf. Figure 47(b)). This proves (3.32). Now we discuss $\beta < 0$. We start with $0 < |\beta| < a$. Then (3.42) exhibits two solutions $\kappa_2(\beta) = 0$,

$0 < \kappa_3(\beta) < \kappa_1(\beta)$. Concerning nonnegative energies we first note that due to $0 < |\beta| < a$, $\cot(ka/2) = -2/\beta k$ has no solutions in $(0, \pi/a)$ since $\tan(x) > x$ for $x \in (0, \pi/2)$. All solutions of (3.37) and (3.38) are now given by $k_n = n\pi/a$, $n \in \mathbb{N}_0$, and, due to the strict monotonicity of $\cot(ka/2)$ and $\cot[(ka + \pi)/2]$ mentioned above, by precisely one additional solution in every interval $(n\pi/a, (n + 1)\pi/a)$, $n \in \mathbb{N}$ (cf. Figure 47(c)). This proves (3.33) for $0 < |\beta| < a$. At $\beta = -a$, $\Xi_{-a,\Lambda}(0)$ has a zero-energy eigenvalue of multiplicity two (cf. the remark after (3.42)). The remaining eigenvalues are obtained identically as in the case $0 < |\beta| < a$. For $|\beta| > a$, (3.42) implies one solution $\kappa_2(\beta) = 0$. The only change compared to the qualitative discussion of the nonnegative eigenvalues in the case $\beta = -a$ now concerns the degeneracy mentioned above. Since $|\beta| > a$, $\cot(ka/2) = -2/\beta k$ now has precisely one solution in $(0, \pi/a)$ and hence this degeneracy is removed (cf. Figure 47(d)). Thus (3.33) is proved. ■

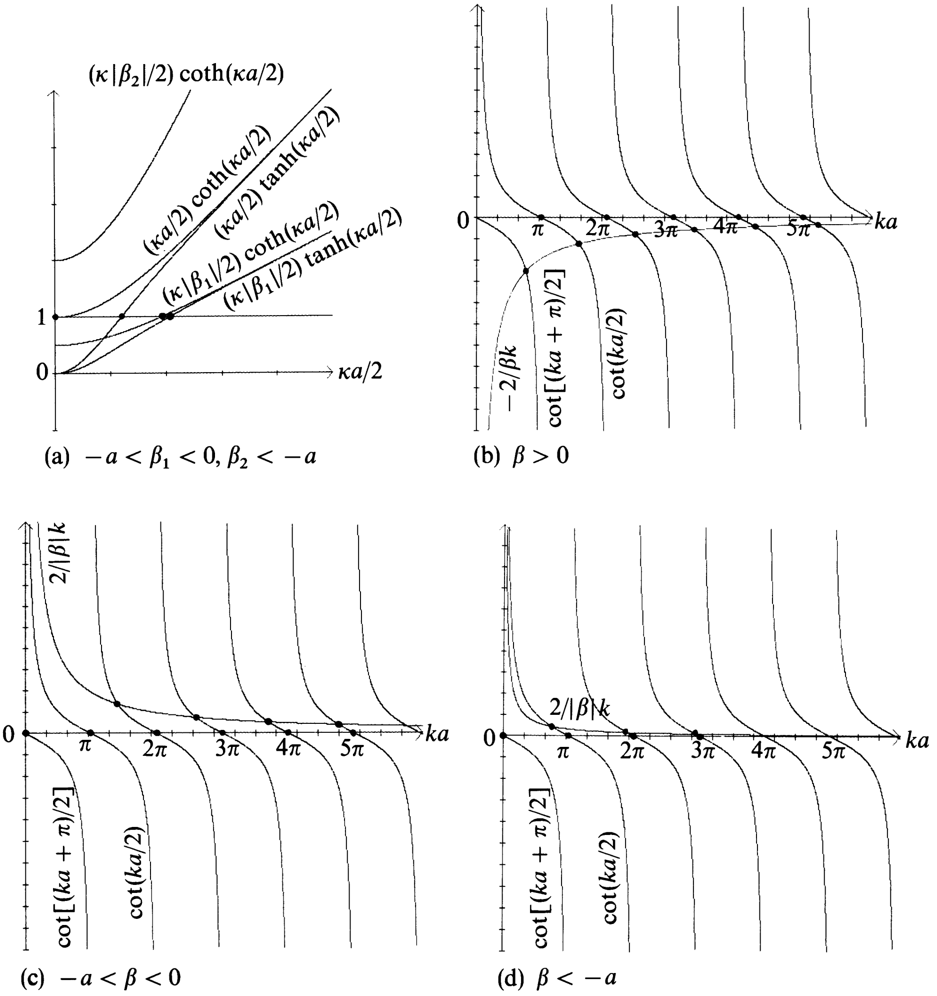


Figure 47

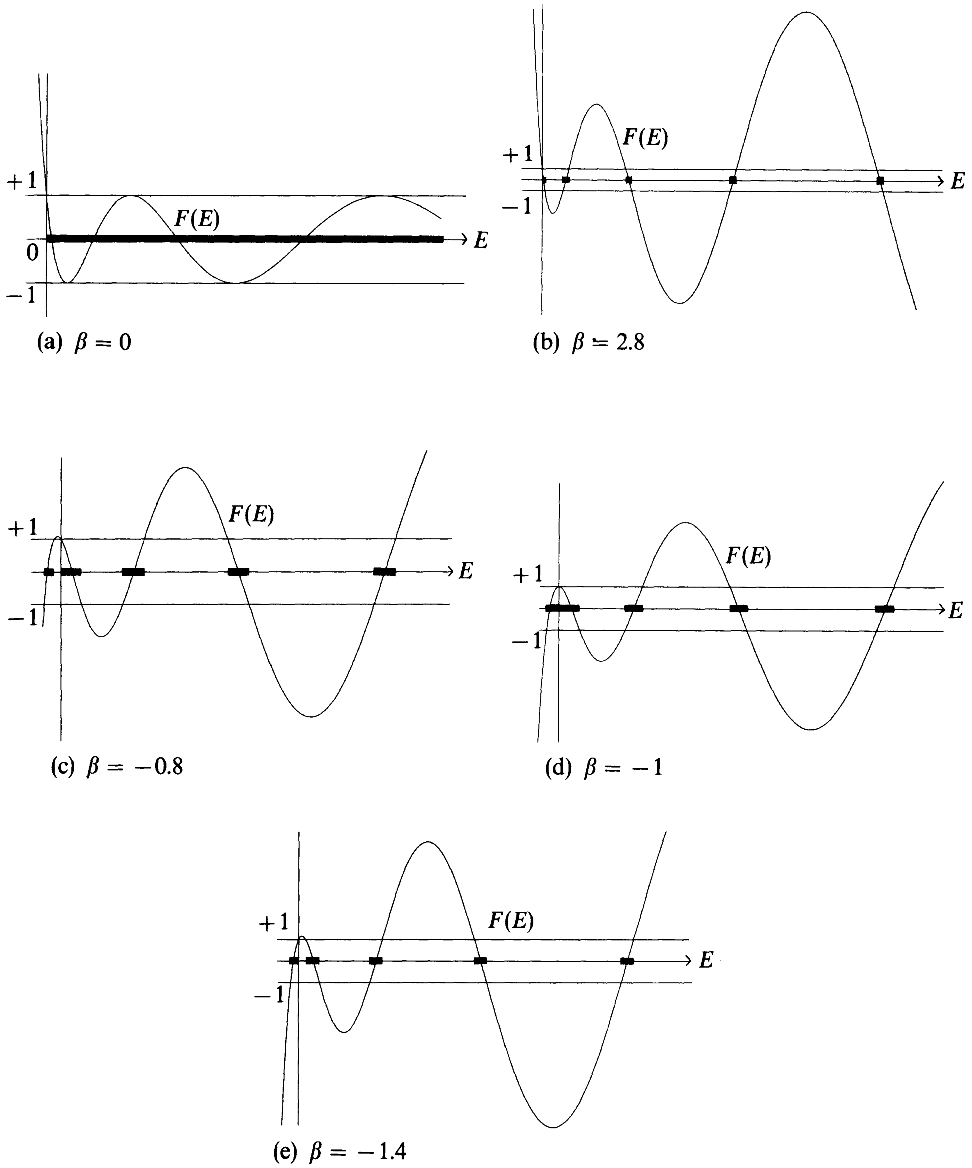


Figure 48 $F(E) = \cos(\sqrt{E}) - (\beta\sqrt{E}/2)\sin(\sqrt{E})$, $\operatorname{Im}\sqrt{E} \geq 0$.

In Figure 48 the right-hand side of (3.29) is plotted as a function of $E = k^2$ ($a = 1$). Whenever $F(E)$ lies in $[-1, 1]$ for some E one can find a $\theta \in \hat{\Lambda}$ such that $\cos(\theta) = F(E)$ and we observe the familiar band structure with infinitely many gaps.

For a plot of $E_m^{\beta,\Lambda}(\theta)$ cf. Figures 49 and 50.

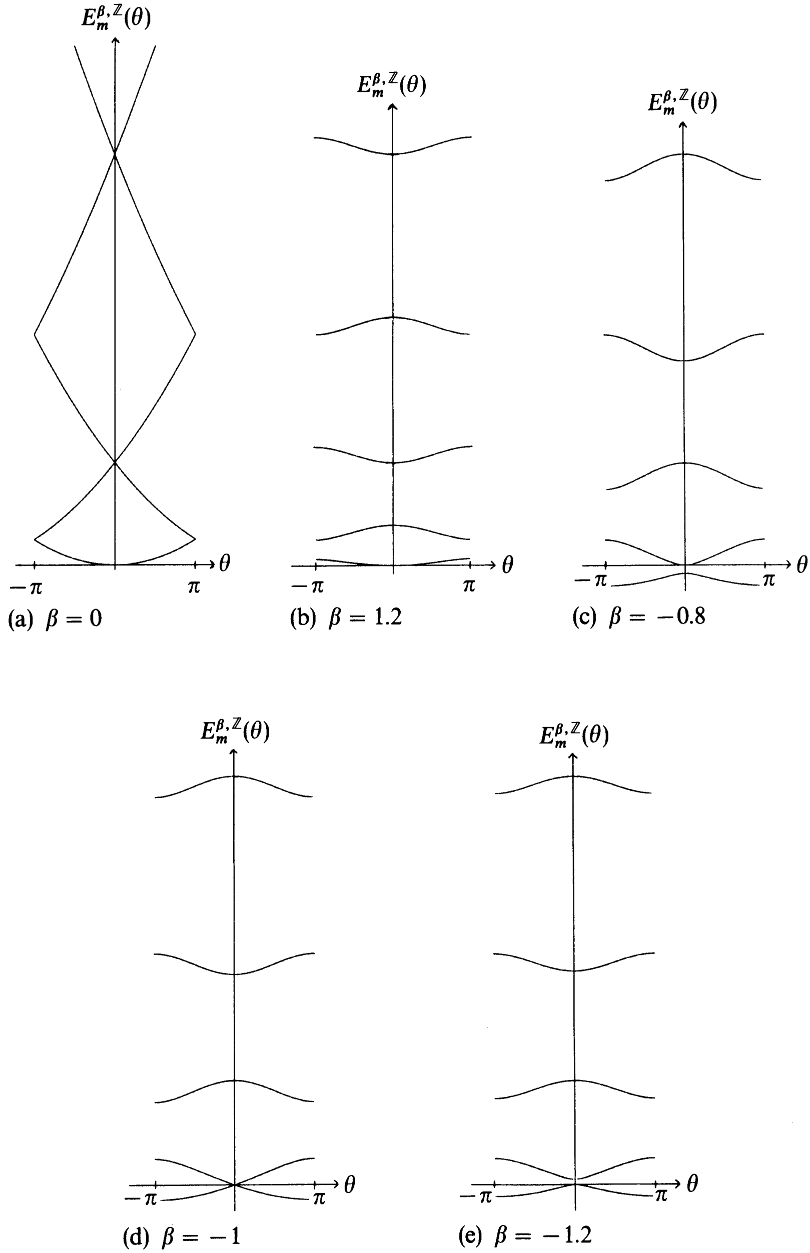


Figure 49 The eigenvalues $E_m^{\beta,\mathbb{Z}}(\theta) = [k_m^{\beta,\mathbb{Z}}(\theta)]^2$, $m = 1, \ldots, 5$, of $\Xi_{\beta,\mathbb{Z}}(\theta)$ as a function of θ, $-\pi \leq \theta < \pi$.

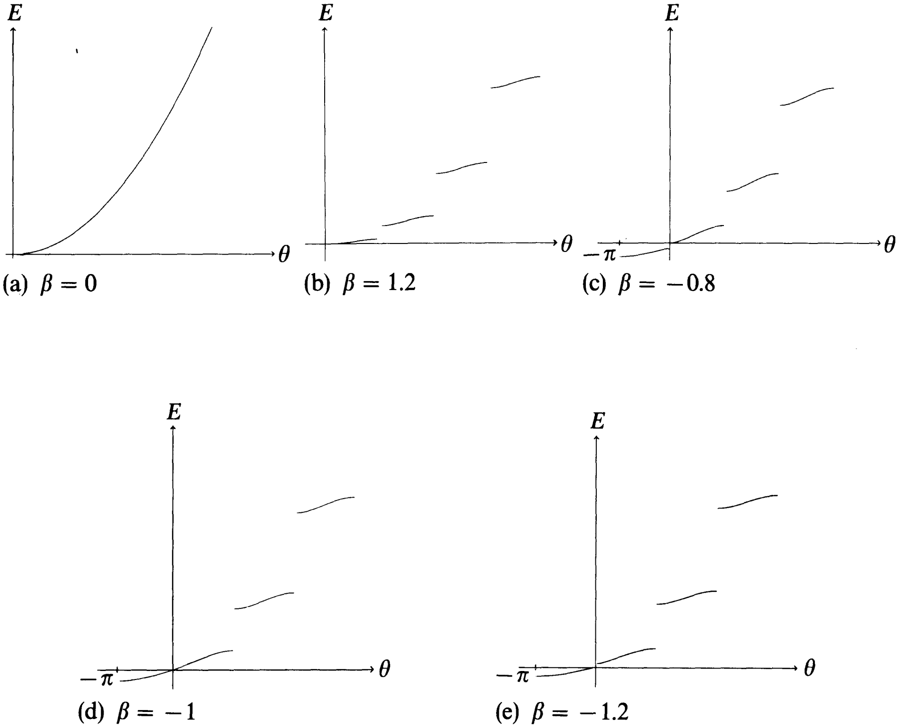


Figure 50 The energy $E = k^2$ as a function of $\theta \geq 0$ for $\beta = 0, 1.2$ and of $\theta \geq -\pi$ for $\beta = -0.8, -1, -1.2$.

In complete analogy to Theorem 2.3.2 we now get

Theorem 3.5. *Let $-\infty < \beta \leq \infty$ and $\Lambda = a\mathbb{Z}$, $a > 0$. Then*

$$\tilde{\mathscr{U}} \Xi_{\beta,\Lambda} \tilde{\mathscr{U}}^{-1} = \int_{[-b/2,b/2)}^{\oplus} \frac{d\theta}{b} \Xi_{\beta,\Lambda}(\theta). \tag{3.43}$$

The analog of Theorem 2.3.3 now reads

Theorem 3.6. *Let $\beta \in \mathbb{R}$ and $\Lambda = a\mathbb{Z}$, $a > 0$. The $\Xi_{\beta,\Lambda}$ has purely absolutely continuous spectrum*

$$\sigma(\Xi_{\beta,\Lambda}) = \sigma_{ac}(\Xi_{\beta,\Lambda}) = \bigcup_{m=1}^{\infty} [a_m^{\beta,\Lambda}, b_m^{\beta,\Lambda}], \qquad a_m^{\beta,\Lambda} < b_m^{\beta,\Lambda} \leq a_{m+1}^{\beta,\Lambda}, \quad m \in \mathbb{N},$$

$$\sigma_{sc}(\Xi_{\beta,\Lambda}) = \varnothing, \qquad \sigma_p(\Xi_{\beta,\Lambda}) = \varnothing. \tag{3.44}$$

Here for $\beta > 0$

$$a_m^{\beta,\Lambda} = \begin{cases} E_m^{\beta,\Lambda}(0) = (m-1)^2\pi^2/a^2, & m \text{ odd}, \\ E_m^{\beta,\Lambda}(-b/2) = (m-1)^2\pi^2/a^2, & m \text{ even}, \end{cases}$$
$$b_m^{\beta,\Lambda} = \begin{cases} E_m^{\beta,\Lambda}(-b/2), & m \text{ odd} \\ E_m^{\beta,\Lambda}(0), & m \text{ even}, \end{cases} \qquad b_m^{\beta,\Lambda} < m^2\pi^2/a^2; \quad m \in \mathbb{N}, \tag{3.45}$$

and for $\beta < 0$

$$a_1^{\beta,\Lambda} = E_1^{\beta,\Lambda}(-b/2) < 0, \qquad a_2^{\beta,\Lambda} = E_2^{\beta,\Lambda}(0)\begin{cases} =0, & |\beta| \le a, \\ >0, & |\beta| > a, \end{cases}$$
$$a_m^{\beta,\Lambda} = \begin{cases} E_m^{\beta,\Lambda}(-b/2), & m \text{ odd}, \\ E_m^{\beta,\Lambda}(0), & m \text{ even}, \end{cases} \qquad m \in \mathbb{N},$$
$$a_m^{\beta,\Lambda} > (m-2)^2\pi^2/a^2, \qquad m \ge 2, \tag{3.46}$$
$$b_1^{\beta,\Lambda} = E_1^{\beta,\Lambda}(0)\begin{cases} <0, & |\beta| < a, \\ =0, & |\beta| \ge a, \end{cases}$$
$$b_m^{\beta,\Lambda} = \begin{cases} E_m^{\beta,\Lambda}(0) = (m-1)^2\pi^2/a^2, & m \text{ odd}, \\ E_m^{\beta,\Lambda}(-b/2) = (m-1)^2\pi^2/a^2, & m \text{ even}, \end{cases} \qquad m = 2, 3 \ldots,$$

with $E_m^{\beta,\Lambda}(\theta)$ the eigenvalues of $\Xi_{\beta,\Lambda}(\theta)$ described in Theorem 3.4. As $m \to \infty$ the length of the mth gap $a_{m+1}^{\beta,\Lambda} - b_m^{\beta,\Lambda}$ resp. the width of the mth band $b_m^{\beta,\Lambda} - a_m^{\beta,\Lambda}$ asymptotically fulfill

$$a_{m+1}^{\beta,\Lambda} - b_m^{\beta,\Lambda} \underset{m\to\infty}{=} 2m\pi^2 a^{-2} - [(8a/|\beta|) + \pi^2]a^{-2} + (8/a\beta m) + O(m^{-2}),$$
$$b_m^{\beta,\Lambda} - a_m^{\beta,\Lambda} \underset{m\to\infty}{=} (8/a|\beta|) - (8/a\beta m) + O(m^{-2}). \tag{3.47}$$

For $\beta \in \mathbb{R} - \{0\}$, $\Xi_{\beta,\Lambda}$ has infinitely many gaps in its spectrum. Since $E_m^{\beta,\Lambda}(0)$, $E_m^{\beta,\Lambda}(-b/2)$, $m \in \mathbb{N}$, are simple for $\beta \ne -a$, all possible gaps in $\sigma(\Xi_{\beta,\Lambda})$ occur in this case. For $\beta = -a$, $\Xi_{-a,\Lambda}(0)$ has a degenerate zero-energy eigenvalue and thus the first gap closes at zero. Due to the simplicity of $E_m^{-a,\Lambda}(0)$, $m \ge 2$, and $E_m^{-a,\Lambda}(-b/2)$, $m \in \mathbb{N}$, all other possible gaps do actually occur. For $\beta = 0$, $\Xi_{0,\Lambda}$ equals $-\Delta$ on $H^{2,2}(\mathbb{R})$ and due to the degeneracy of $E_m^{0,\Lambda}(0)$, $m \ge 2$, and $E_m^{0,\Lambda}(-b/2)$, $m \in \mathbb{N}$, all gaps close (cf. (2.3.37)). For $\beta = \infty$, $\Xi_{\infty,\Lambda}$ equals the Neumann Laplacian on $\mathbb{R} - \Lambda$ and hence reduces to an infinite direct sum of Neumann Laplacians on $(ma, (m+1)a)$, $m \in \mathbb{Z}$. Thus its spectrum is pure point with each eigenvalue of infinite multiplicity

$$\sigma_c(\Xi_{\infty,\Lambda}) = \varnothing,$$
$$\sigma_{ess}(\Xi_{\infty,\Lambda}) = \sigma_p(\Xi_{\infty,\Lambda}) = \{m^2\pi^2/a^2 \mid m \in \mathbb{N}_0\}. \tag{3.48}$$

Furthermore, we note a strict monotonicity of $\sigma(\Xi_{\beta,\Lambda})$ with respect to β (being a consequence of the monotonicity of $E_m^{\beta,\Lambda}(0)$, $E_m^{\beta,\Lambda}(-b/2)$, $m \in \mathbb{N}$, *with respect to* $\beta \in \mathbb{R}$ *as mentioned in Theorem* 3.4)

$$\begin{aligned} \sigma(\Xi_{\beta,\Lambda}) &\subset \sigma(\Xi_{\beta',\Lambda}), & 0 &\le \beta' < \beta, \\ \sigma(\Xi_{\beta,\Lambda}) &\supset \sigma(\Xi_{\beta',\Lambda}), & -\infty &\le \beta' < \beta \le -a. \end{aligned} \tag{3.49}$$

The band edges $a_m^{\beta,\Lambda}$, $b_m^{\beta,\Lambda}$, $m \in \mathbb{N}$, *are continuous with respect to* $\beta \in \mathbb{R}$.

PROOF. Since one can follow the proof of Theorem 2.3.3 step by step we omit any details. ■

The spectrum of $\Xi_{\beta,\Lambda}$ as a function of the coupling constant $\beta \in \mathbb{R}$ is illustrated in Figure 51.

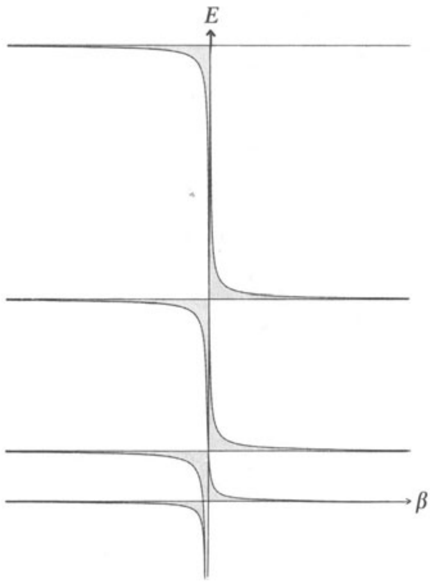


Figure 51 The band spectrum of $\Xi_{\beta,\mathbb{Z}}$ as a function of β (cf. also Figures 49 and 50).

We would like to stress the curious fact that for $\beta < 0$ the lower band edges of $\Xi_{\beta,\Lambda}$ are given by $E_m^{\beta,\Lambda}(-b/2)$, i.e., by the antiperiodic eigenvalues and not by the periodic eigenvalues $E_m^{\beta,\Lambda}(0)$. The reason for this is clear from (3.36) since the discriminant behaves atypical as $E = -\kappa^2 \to -\infty$ for $\beta < 0$, viz.

$$\lim_{\kappa\to\infty} [\cosh(\kappa a) + (\beta\kappa/2)\sinh(\kappa a)] = \begin{cases} +\infty, & \beta \ge 0, \\ -\infty, & \beta < 0. \end{cases} \tag{3.50}$$

This phenomenon is connected with the fact that $\Xi_{\beta,\Lambda}(0)$ has a ground state which changes sign for $v \lessgtr 0$. Hence the usual positivity preserving arguments (cf. the proof of Theorem XIII.89e in [391]) break down.

The density of states $d\rho^{\beta,\Lambda}/dE$ of $\Xi_{\beta,\Lambda}$ at a point $E = k^2$ with $E_m^{\beta,\Lambda}(\theta) = E$,

$m \in \mathbb{N}$, is then given by

$$\frac{d\rho^{\beta,\Lambda}}{dE} = \frac{1}{2\pi k}\frac{d\theta}{dk} = \frac{\operatorname{sgn}(\beta)}{2\pi|k|}\frac{|\sin(ka)|}{|\sin(\theta a)|}\{1 + (\beta/2a)[1 + ka\cot(ka)]\},$$
$$\operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad k^2 \in \mathring{\sigma}(\Xi_{\beta,\Lambda}). \quad (3.51)$$

Here $\theta = \theta(k)$ is extended from 0 to ∞ for $\beta \geq 0$ and from $-\pi/a$ to ∞ for $\beta < 0$:

$$\theta(k) = (-1)^{m+1}a^{-1}\arccos[\cos(ka) - (\beta k/2)\sin(ka)] + \begin{cases} m\pi/a, & m \text{ odd}, \\ (m-1)\pi/a, & m \text{ even}, \end{cases}$$
$$\beta \geq 0, \quad k^2 \in (a_m^{\beta,\Lambda}, b_m^{\beta,\Lambda}), \quad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad m \in \mathbb{N}, \quad (3.52)$$

$$\theta(k) = (-1)^{m}a^{-1}\arccos[\cos(ka) - (\beta k/2)\sin(ka)] + \begin{cases} (m-1)\pi/a, & m \text{ odd}, \\ (m-2)\pi/a, & m \text{ even}, \end{cases}$$
$$\beta < 0, \quad k^2 \in (a_m^{\beta,\Lambda}, b_m^{\beta,\Lambda}), \quad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \quad m \in \mathbb{N}. \quad (3.53)$$

Again the density of states behaves like $d\rho^{\beta,\Lambda}/dE = O(|E - E_m|^{-1/2})$ near the band edges $E_m \in \{a_m^{\beta,\Lambda}, b_m^{\beta,\Lambda}\}_{m\in\mathbb{N}}$.

Next we briefly indicate how to construct the resolvent of $\Xi_{\beta,\Lambda}(\theta)$ in momentum space. Similar to the corresponding two- and three-dimensional problem (and in contrast to the Kronig–Penney situation in (2.3.49)–(2.3.56)) this approach requires a certain renormalization procedure. We start with the operator in $l^2(\Gamma)$ (cf. also the end of Appendix G)

$$(\hat{H}^\omega(\theta)g)(\gamma) = (\gamma + \theta)^2 g(\gamma) + \mu^\omega(\chi_\omega(\cdot + \theta)(\cdot + \theta), g)\chi_\omega(\gamma + \theta)(\gamma + \theta),$$
$$\gamma \in \Gamma, \quad \omega > 0,$$

$$g \in \mathscr{D}(\hat{H}^\omega(\theta)) = \left\{g \in l^2(\Gamma) \,\middle|\, \sum_{\gamma\in\Gamma}(\gamma + \theta)^4|g(\gamma)|^2 < \infty\right\}, \qquad \theta \in \hat{\bar{\Lambda}}, \qquad (3.54)$$

and $\chi_\omega(\cdot)$ has been defined in (2.3.50). From Lemma B.5 we infer that

$$(\hat{H}^\omega(\theta) - k^2)^{-1}$$
$$= G_k(\theta) - [(\mu^\omega)^{-1} + (\chi_\omega(\cdot + \theta)(\cdot + \theta), G_k(\theta)\chi_\omega(\cdot + \theta)(\cdot + \theta))]^{-1} \cdot$$
$$\cdot\overline{(G_k(\theta)\chi_\omega(\cdot + \theta)(\cdot + \theta)}, \cdot)G_k(\theta)\chi_\omega(\cdot + \theta)(\cdot + \theta), \quad \theta \in \hat{\bar{\Lambda}}, \quad (3.55)$$

where $G_k(\theta)$ has been defined in (2.3.52). Since

$$(\chi_\omega(\cdot + \theta)(\cdot + \theta), G_k(\theta)\chi_\omega(\cdot + \theta)(\cdot + \theta)) = \sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\leq\omega}} \frac{(\gamma + \theta)^2}{(\gamma + \theta)^2 - k^2}$$

$$= 2\begin{Bmatrix} \left[\left[\dfrac{\omega a}{2\pi}\right]\right], & \theta \in \hat{\bar{\Lambda}} - \{0\} \\ \left[\left[\dfrac{\omega a}{2\pi}\right]\right] + 1, & \theta = 0 \end{Bmatrix} + k^2 \sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\leq\omega}} \frac{1}{(\gamma + \theta)^2 - k^2} \quad (3.56)$$

we choose the renormalized coupling constant to be

$$(\mu^{\omega})^{-1} = -2\left\{\begin{matrix} \left[\left[\dfrac{\omega a}{2\pi}\right]\right], & \theta \in \hat{\bar{\Lambda}} - \{0\} \\ \left[\left[\dfrac{\omega a}{2\pi}\right]\right] + 1, & \theta = 0 \end{matrix}\right\} - a\beta^{-1}, \qquad -\infty < \beta \leq \infty. \tag{3.57}$$

(Here $[[x]]$ denotes the integer part of x, cf. Sect. 2.6.) Thus we get the final result

$$\begin{aligned} \text{n-}\lim_{\omega\to\infty} (\hat{H}^{\omega}(\theta) - k^2)^{-1} &\equiv (\hat{\Xi}_{\beta,\Lambda}(-\theta) - k^2)^{-1} \\ &= G_k(\theta) - (\beta/a)\frac{\cos(ka) - \cos(\theta a)}{\cos(\theta a) - \cos(ka) + (\beta k/2)\sin(ka)}(\overline{\tilde{F}_k(\theta)}, \cdot)\tilde{F}_k(\theta), \\ &k^2 \in \rho(\hat{\Xi}_{\beta,\Lambda}(-\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\bar{\Lambda}}, \quad -\infty < \beta \leq \infty, \end{aligned} \tag{3.58}$$

where

$$\begin{aligned} \tilde{F}_k(\theta)(\gamma) &= ((\gamma + \theta)^2 - k^2)^{-1}(\gamma + \theta), \\ &k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\bar{\Lambda}}, \quad \gamma \in \Gamma. \end{aligned} \tag{3.59}$$

The rest of Sect. 2.3 now goes through in the δ'-case as in the δ-case, since due to the similarity of (3.17) (resp. (3.24)) and (2.1.49) (resp. (2.1.55)) one model can be transformed into the other by the substitution

$$(\alpha_j/k) \leftrightarrow -\beta_j k, \qquad j \in \mathbb{Z}, \tag{3.60}$$

keeping Y fixed. As an example of this substitution we mention, e.g., the analog of Theorem 2.3.6.

Theorem 3.7. *Let $\beta = \{\beta_j\}_{j\in\mathbb{Z}}$ be a bounded sequence of real numbers, $\Lambda = a\mathbb{Z}$, $a > 0$, and assume U to be open. If*

$$U \subseteq \bigcap_{j\in\mathbb{Z}} \rho(\Xi_{\beta_j,\Lambda}) \quad \text{then} \quad U \subseteq \rho(\Xi_{\beta,\Lambda}). \tag{3.61}$$

Since the analog of Lemma 2.3.6 for δ'-interactions also trivially holds we omit further details and turn directly to *half-crystals*. We assume the notations (2.4.1) and (2.4.2) except that we replace the symbol α by β to obtain consistency with our earlier treatment in this chapter. Then the analog of Theorem 2.4.1 for the spectrum of $\Xi_{\beta^{-+},\Lambda}$ is obviously true and hence we pass immediately to the analog of Theorem 2.4.2. Again we rely on the difference equation (3.24). Since now $\psi_j(k) = \psi'(k, ja)$ (in contrast to Sect. 2.4 where $\psi_j(k) = \psi(k, ja)$) the analog of the ansatz (2.4.5) and (2.4.9) now reads

$$\psi_j^+ = \begin{cases} N_-[e^{i\theta_- aj} - e^{-i\theta_- aj}\tilde{\mathscr{R}}^1], & j = -1, -2, \ldots, \\ N_+ e^{i\theta_+ aj}\tilde{T}^1, & j = 0, 1, 2, \ldots, \quad \operatorname{Im}\theta_\pm \geq 0, \end{cases} \tag{3.62}$$

$$\psi_j^- = \begin{cases} M_+[e^{-i\theta_+ aj} - e^{i\theta_+ aj}\tilde{\mathscr{R}}^{\mathrm{r}}], & j = 0, 1, 2, \ldots, \\ M_- e^{-i\theta_- aj}\tilde{T}^{\mathrm{r}}, & j = -1, -2, \ldots, \quad \operatorname{Im}\theta_\pm \geq 0. \end{cases} \tag{3.63}$$

As in Sect. 2.4, (3.24), (3.62), and (3.63) in the cases $j \leq -2$ and $j \geq 1$ immediately lead to

$$\cos(\theta_\mp a) = (\varepsilon - \mu^\mp)/2, \qquad \operatorname{Im}\theta_\mp \geq 0, \tag{3.64}$$

where now

$$\varepsilon = 2\cos(ka), \qquad \mu_j = \begin{cases} \mu^+, & j = 0, 1, 2, \ldots, \\ \mu^-, & j = -1, -2, \ldots, \end{cases} \qquad \mu^\pm = \beta^\pm k \sin(ka),$$
$$k \neq m\pi/a, \quad m \in \mathbb{Z}. \tag{3.65}$$

The rest of the calculation is thus identical to that in Sect. 2.4: In fact, formulas (2.4.23)–(2.4.32) directly apply in the present δ'-case if $\mathscr{R}^{\mathrm{l(r)}}$ are replaced by $-\mathscr{R}^{\mathrm{l(r)}}$ in (2.4.24), (2.4.28), and (2.4.31) (cf. (3.62) and (3.63)) and $\alpha^\pm$ by $-\beta^\pm k^2$ in (2.4.25), (2.4.29), and (2.4.32). (Actually, the replacement $\mathscr{R}^{\mathrm{l(r)}} \to -\mathscr{R}^{\mathrm{l(r)}}$ and $\alpha \to -\beta k^2$ in the N-center scattering matrix (II.2.4.7) of $-\Delta_{\alpha,Y}$ immediately yields the N-center scattering matrix (II.3.31) of $\Xi_{\beta,Y}$.) The reason behind the substitution $\alpha \to -\beta k^2$ is of course the fact that

$$\Gamma_{-\beta k^2, Y}(k) = -\tilde{\Gamma}_{\beta,Y}(k), \qquad \operatorname{Im} k > 0, \tag{3.66}$$

where $\Gamma_{\alpha,Y}(k)$ (resp. $\tilde{\Gamma}_{\alpha,Y}(k)$) are defined in (2.1.18) (resp. (3.7)).

Finally, we turn to the analog of Sect. 2.6, i.e., to *defects* and *impurity scattering* in the context of δ'-crystals. We replace $-\Delta_{\alpha,Y}$ in (2.6.1) by $\Xi_{\beta,Y}$ and at the same time $-\Delta_{\alpha,Y,\gamma,Z}$ in obvious notation by $\Xi_{\beta,Y,\gamma,Z}$ (in particular, all additional interactions of strength γ_l at the impurity points $z_l \in Z$, $l = 1, \ldots, M$, are represented by δ'-boundary conditions so that no mixture of δ- and δ'-interactions occurs). Then Theorems 2.6.1 and 2.6.2 immediately extend to the δ'-case. In fact, using again the above trick that the first derivative of a wave function corresponding to a system of δ-interactions described, e.g., by $-\Delta_{\alpha,Y}$ is proportional to the corresponding wave function of $\Xi_{\beta,Y}$ if after differentiation α is replaced by $-\beta k^2$ (i.e., $\alpha_j \to -\beta_j k^2$ for all $j \in J$) reproduces all results of Sect. 2.6 for the present δ'-case. As a simple example we give the Bloch wave function associated with $\Xi_{\beta,\Lambda}$ (i.e., the analog of (2.6.11)). In fact,

$$\Psi_{\beta,\Lambda}(k, \sigma, x)$$
$$= \Psi'_{\beta,\Lambda}(k, \sigma, 0)(\beta/2)e^{i\theta\sigma x}e^{-i\theta\sigma x'}\left\{\frac{e^{i\theta\sigma a}\cos(kx') - \cos[k(x' - a)]}{\cos(\theta a) - \cos(ka)}\right\},$$
$$x' = x - a[[x/a]], \quad x \in \mathbb{R}, \quad \operatorname{Im} k \geq 0, \quad \sigma = \pm 1, \quad \operatorname{Im}\theta \geq 0, \quad \operatorname{Re}\theta \geq 0, \tag{3.67}$$

satisfies

$$-\Psi''_{\beta,\Lambda}(k, \sigma, x) = k^2 \Psi_{\beta,\Lambda}(k, \sigma, x),$$
$$\operatorname{Im} k \geq 0, \quad \sigma = \pm 1, \quad x \in \mathbb{R} - \Lambda, \tag{3.68}$$

and the boundary conditions

$$\Psi'_{\beta,\Lambda}(k, \sigma, na+) = \Psi'_{\beta,\Lambda}(k, \sigma, na-),$$
$$\Psi_{\beta,\Lambda}(k, \sigma, na+) - \Psi_{\beta,\Lambda}(k, \sigma, na-) = \beta\Psi'_{\beta,\Lambda}(k, \sigma, na),$$
$$\operatorname{Im} k \geq 0, \quad \sigma = \pm 1, \quad n \in \mathbb{N}. \tag{3.69}$$

Taking the left (or right) derivative at $x = 0$ in (3.67) immediately yields (3.2.9). Since x' is periodic with period a, (3.67) indeed represents a Bloch wave. The analogs of the remaining results in Sect. 2.6 are now a simple exercise of the above-mentioned substitution $\alpha \to -\beta k^2$ (bearing in mind that reflection coefficients in (2.6.51) and (2.6.52) pick up an additional minus sign, as is clear from the discussion after (3.65)).

Notes

The results of this chapter are taken from Gesztesy, Holden, and Kirsch [205], [206].

CHAPTER III.4

Infinitely Many Point Interactions in Two Dimensions

The presentation in this chapter is modeled after the three-dimensional case, Ch. 1. In order to make the presentation short, we will concentrate on the existence of $-\Delta_{\alpha,Y}$ when

$$Y = \{y_j | j \in \mathbb{N}\} \subset \mathbb{R}^2 \tag{4.1}$$

with

$$\inf_{\substack{j \neq j' \\ j,j' \in \mathbb{N}}} |y_j - y_{j'}| = d > 0 \tag{4.2}$$

and on the crystal and the polymer where we explicitly compute the spectrum. The existence theorem now reads

Theorem 4.1. *Let $Y = \{y_j | j \in \mathbb{N}\} \subset \mathbb{R}^2$ be discrete in the sense of* (4.2) *and let α: $Y \to \mathbb{R}$. Then the strong limit*

$$\underset{\substack{\tilde{Y} \subset Y \\ |\tilde{Y}| < \infty}}{\text{s-lim}} (-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \tag{4.3}$$

over the filter of all finite subsets $\tilde{Y}$ of Y exists, where $\tilde{\alpha} = \alpha|_{\tilde{Y}}$ and $(-\Delta_{\tilde{\alpha},\tilde{Y}} - k^2)^{-1}$ is given by (II.4.22). *The limit equals the resolvent of a self-adjoint operator $-\Delta_{\alpha,Y}$ which has the resolvent*

$$(-\Delta_{\alpha,Y} - k^2)^{-1} = G_k + \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1} (\overline{G_k(\cdot - y_{j'})}, \cdot) G_k(\cdot - y_j),$$

$$k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \text{Im}\, k > 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j \in \mathbb{N}, \tag{4.4}$$

where $\Gamma_{\alpha,Y}(k)$ is the closed operator in $l^2(Y)$ given by

$$\Gamma_{\alpha,Y}(k) = \left[\left(\alpha_j - \frac{1}{2\pi}(\Psi(1) - \ln(k/2i))\right)\delta_{jj'} - \tilde{G}_k(y_j - y_{j'})\right]_{j,j' \in \mathbb{N}},$$
$$\operatorname{Im} k \geq 0, \quad (4.5)$$

and

$$\tilde{G}_k(x) = \begin{cases} G_k(x), & x \neq 0, \\ 0, & x = 0, \end{cases} \qquad G_k(x) = (i/4)H_0^{(1)}(k|x|), \quad x \neq 0, \quad \operatorname{Im} k \geq 0. \quad (4.6)$$

We have

$$[\Gamma_{\alpha,Y}(k)]^{-1} \in \mathscr{B}(l^2(Y)), \qquad k^2 \in \rho(-\Delta_{\alpha,Y}), \quad \operatorname{Im} k > 0 \quad \text{large enough.} \quad (4.7)$$

If α is bounded, then $\Gamma_{\alpha,Y}(k)$ is analytic in k for $\operatorname{Im} k > 0$. *Let*

$$-\hat{\Delta}_{\alpha,Y} = \mathscr{F}[-\Delta_{\alpha,Y}]\mathscr{F}^{-1}, \quad (4.8)$$

where $\mathscr{F}$ is the Fourier transform,

$$\mathscr{F}\colon L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2),$$

$$(\mathscr{F}f)(p) = \operatorname*{s-lim}_{R\to\infty} (2\pi)^{-1} \int_{|x|\leq R} d^2x\, f(x)e^{-ipx}, \qquad f \in L^2(\mathbb{R}^2). \quad (4.9)$$

Then $-\hat{\Delta}_{\alpha,Y}$ has the resolvent

$$(\hat{g}, (-\hat{\Delta}_{\alpha,Y} - k^2)^{-1}\hat{f}) = (\hat{g}, (p^2 - k^2)^{-1}\hat{f})$$
$$+ \sum_{j,j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]_{jj'}^{-1}(\hat{g}, F_{k,y_j})(F_{-\bar{k},y_{j'}}, \hat{f}),$$

$$k^2 \in \rho(-\hat{\Delta}_{\alpha,Y}), \quad \operatorname{Im} k > 0, \quad \alpha_j \in \mathbb{R}, \quad y_j \in Y, \quad j \in \mathbb{N}, \quad \hat{f}, \hat{g} \in L^2(\mathbb{R}^2), \quad (4.10)$$

where

$$F_{k,y_j}(p) = (2\pi)^{-1}\frac{e^{-ipy_j}}{p^2 - k^2}, \qquad p \in \mathbb{R}^2, \quad y_j \in Y, \quad j \in \mathbb{N}. \quad (4.11)$$

Proof. The proof is similar to that of Theorem 1.1.1 since we still have the estimate

$$|G_k(x)| \leq ce^{-\operatorname{Im} k|x|}, \qquad \operatorname{Im} k > 0, \quad (4.12)$$

for large $|x|$ and some constant $c > 0$ ([1], p. 378). ■

The explicit characterization of the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ and the locality property still carries over to the case of infinitely many centers, as the next theorem shows.

Theorem 4.2. *Let $y_j \in Y$, $|y_j - y_{j'}| \geq d > 0$, $\alpha_j \in \mathbb{R}$, $j \neq j'$, $j, j' \in \mathbb{N}$. Then the domain $\mathscr{D}(-\Delta_{\alpha,Y})$ of $-\Delta_{\alpha,Y}$ consists of all functions ψ such that*

$$\psi(x) = \phi_k(x) + \sum_{j=1}^{\infty} a_j(k)G_k(x - y_j), \qquad x \in \mathbb{R}^2 - Y, \quad (4.13)$$

for some k with Im $k > 0$ *where*

$$\phi_k \in \mathscr{D}(-\Delta) = H^{2,2}(\mathbb{R}^2), \qquad a_j(k) = \sum_{j'=1}^{\infty} [\Gamma_{\alpha,Y}(k)]^{-1}_{jj'} \phi_k(y_{j'}), \qquad j \in \mathbb{N}. \tag{4.14}$$

Furthermore, this decomposition is unique,

$$(-\Delta_{\alpha,Y} - k^2)\psi = (-\Delta - k^2)\phi_k, \tag{4.15}$$

and if $\psi = 0$ *in some open domain* $U \subseteq \mathbb{R}^2$, *then also* $-\Delta_{\alpha,Y}\psi = 0$ *in* U.

PROOF. Similar to that of Theorem 1.1.2. ∎

We now turn directly to the periodic case, i.e., we will analyze the one-electron model of a two-dimensional crystal with point interactions. The general discussion of Sect. 1.3 is, except for normalization constants, still valid, and our presentation will follow the first part of Sect. 1.4. First, we have to introduce the basic quantities. Let Λ be a Bravais lattice, i.e.,

$$\Lambda = \{n_1 a_1 + n_2 a_2 \in \mathbb{R}^2 | (n_1, n_2) \in \mathbb{Z}^2\}, \tag{4.16}$$

a_1 and a_2 being two linearly independent vectors in $\mathbb{R}^2$. The dual lattice Γ is given by

$$\Gamma = \{n_1 b_1 + n_2 b_2 \in \mathbb{R}^2 | (n_1, n_2) \in \mathbb{Z}^2\}, \tag{4.17}$$

where

$$a_j b_{j'} = 2\pi\delta_{jj'}, \qquad j, j' = 1, 2. \tag{4.18}$$

The dual groups $\hat{\Lambda}$, the Brillouin zone, and $\hat{\Gamma}$ equal

$$\hat{\Lambda} = \mathbb{R}^2/\Gamma = \{s_1 b_1 + s_2 b_2 \in \mathbb{R}^2 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2\}, \tag{4.19}$$

$$\hat{\Gamma} = \mathbb{R}^2/\Lambda = \{s_1 a_1 + s_2 a_2 \in \mathbb{R}^2 | s_j \in [-\tfrac{1}{2}, \tfrac{1}{2}), j = 1, 2\}, \tag{4.20}$$

respectively. For simplicity, we specialize to $Y = \{0\}$. Then the analog of (1.4.30) reads

$$(\hat{H}^{\omega}(\theta)g)(\gamma) = |\gamma + \theta|^2 g(\gamma) - |\hat{\Gamma}|^{-1}\mu(\omega)(\phi^{\omega}(\theta), g)\phi^{\omega}(\theta),$$
$$\theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l_0(\Gamma), \quad \omega > 0, \tag{4.21}$$

where

$$\phi^{\omega}(\theta, \gamma) = \chi_{\omega}(\theta + \gamma), \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma \tag{4.22}$$

(χ_{ω} being the characteristic function of a closed ball in $\mathbb{R}^2$ with radius ω and center at the origin). The problem is now to choose $\mu(\omega)$ such as to obtain a nontrivial self-adjoint operator in $l^2(\Gamma)$ in the limit $\omega \to \infty$. This is the content of the next

Theorem 4.3. *Let $\hat{H}^{\omega}(\theta)$ be the self-adjoint operator* (4.21) *in $l^2(\Gamma)$ with domain*

$$\mathscr{D}(\hat{H}^{\omega}(\theta)) = \mathscr{D}(-\hat{\Delta}(\theta)) = \left\{ g \in l^2(\Gamma) \,\middle|\, \sum_{\gamma \in \Gamma} |\gamma + \theta|^4 |g(\gamma)|^2 < \infty \right\}, \qquad \theta \in \hat{\Lambda}. \tag{4.23}$$

If

$$\mu(\omega) = \left\{ \alpha - \frac{1}{2\pi}[\Psi(1) + \ln 2 - \ln \omega] \right\}^{-1}, \qquad \alpha \in \mathbb{R}, \quad \omega > 0, \tag{4.24}$$

then $\hat{H}^{\omega}(\theta)$ converges in norm resolvent sense for all $\theta \in \hat{\Lambda}$ as $\omega \to \infty$ to a self-adjoint operator $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ with resolvent

$$\begin{aligned}(-\hat{\Delta}_{\alpha,\Lambda}(\theta) - k^2)^{-1} &\\ = G_k(\theta) + |\hat{\Gamma}|^{-1} &\left[\alpha - \frac{1}{2\pi}\Psi(1) - g_k(\theta) \right]^{-1} (\overline{G_k(\theta, \cdot)}, \cdot) G_k(\theta, \cdot), \\ & k^2 \in \rho(-\hat{\Delta}_{\alpha,\Lambda}(\theta)), \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \quad \alpha \in \mathbb{R}, \end{aligned} \tag{4.25}$$

where

$$\begin{aligned} &G_k(\theta): l^2(\Gamma) \to l^2(\Gamma), \\ &(G_k(\theta)g)(\gamma) = G_k(\theta, \gamma) g(\gamma) = (|\gamma + \theta|^2 - k^2)^{-1} g(\gamma), \\ &k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad g \in l^2(\Gamma), \end{aligned} \tag{4.26}$$

and

$$\begin{aligned} g_k(\theta) = (2\pi)^{-2} \lim_{\omega \to \infty} &\left[\sum_{\substack{\gamma \in \Gamma \\ |\gamma + \theta| \leq \omega}} \frac{|\hat{\Lambda}|}{|\gamma + \theta|^2 - k^2} - 2\pi \ln \omega \right], \\ & k^2 \notin |\Gamma + \theta|^2, \quad \operatorname{Im} k \geq 0, \quad \theta \in \hat{\Lambda}. \end{aligned} \tag{4.27}$$

PROOF. Applying Lemma B.5 we have

$$\begin{aligned} (\hat{H}^{\omega}(\theta) - k^2)^{-1} = G_k(\theta) & \\ - [|\hat{\Gamma}| \mu(\omega)^{-1} &+ (\phi^{\omega}(\theta), G_k(\theta)\phi^{\omega}(\theta))]^{-1} (\overline{G_k(\theta)}\phi^{\omega}(\theta), \cdot) G_k(\theta)\phi^{\omega}(\theta), \\ & k^2 \in \rho(\hat{H}^{\omega}(\theta)), \quad \operatorname{Im} k > 0, \quad \theta \in \hat{\Lambda}. \end{aligned} \tag{4.28}$$

Since

$$\begin{aligned} &|\hat{\Gamma}| \mu(\omega)^{-1} + (\phi^{\omega}(\theta), G_k(\theta)\phi^{\omega}(\theta)) \\ &= |\hat{\Gamma}| \left\{ \alpha - \frac{1}{2\pi}[\Psi(1) + \ln 2] + \frac{1}{2\pi} \ln \omega - (2\pi)^{-2} \sum_{\substack{\gamma \in \Gamma \\ |\gamma + \theta| \leq \omega}} \frac{|\hat{\Lambda}|}{|\gamma + \theta|^2 - k^2} \right\} \\ &\xrightarrow[\omega \to \infty]{} |\hat{\Gamma}| \left[\alpha - \frac{1}{2\pi}\Psi(1) - g_k(\theta) \right] \end{aligned} \tag{4.29}$$

exists due to Lemma 4.4, the rest of the proof is similar to that of Theorem 1.4.1. ■

Also in two dimensions we shall make use of the Poisson summation formula.

Lemma 4.4 (Poisson Summation Formula). *Let $k^2 \in \mathbb{C}$, $\operatorname{Im} k > 0$, and $\theta \in \hat{\Lambda}$. Then*

$$(2\pi)^{-2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\omega}} \frac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - 2\pi \ln \omega \right]$$

$$= \sum_{\substack{\lambda\in\Lambda \\ \lambda\neq 0}} G_k(\lambda) e^{-i\theta\lambda} + \frac{1}{2\pi} \ln(k/i). \quad (4.30)$$

PROOF. Let

$$f(\omega) = \sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\omega}} \frac{1}{|\gamma+\theta|^2 - k^2}, \qquad \omega \ge 0, \quad (4.31)$$

($k \in \mathbb{C}$, $\operatorname{Im} k > 0$, and $\theta \in \hat{\Lambda}$ will be fixed), and define

$$F(\eta) = \int_0^\infty e^{-\omega^2/4\eta}\, df(\omega) = \sum_{\gamma\in\Gamma} \frac{e^{-|\gamma+\theta|/4\eta}}{|\gamma+\theta|^2 - k^2}, \qquad \eta > 0. \quad (4.32)$$

The Poisson summation formula ([94], Theorem 67, and eq. (19), p. 260) then gives

$$F(\eta) = \frac{|\hat{\Gamma}|}{2\pi} 2\eta \int_{\mathbb{R}^2} d^2x\, G_k(x) e^{-\eta x^2} + \frac{|\hat{\Gamma}|}{2\pi} \sum_{\substack{\lambda\in\Lambda \\ \lambda\neq 0}} 2\eta \int_{\mathbb{R}^2} d^2x\, G_k(x-\lambda) e^{-\eta x^2} e^{-i\lambda\theta}$$

$$= |\hat{\Gamma}| \left[\frac{1}{4\pi} \int_0^\infty dt \frac{e^{-t/4\eta}}{t-k^2} + \frac{1}{2\pi} \sum_{\lambda\in\Lambda} \tilde{G}_k(\lambda) e^{-i\lambda\theta} + o(1) \right] \quad \text{as } \eta \to \infty. \quad (4.33)$$

Define

$$\tilde{F}(\eta) = \int_0^\infty e^{-\omega^2/4\eta} d\left[f(\omega) - \frac{\pi}{|\hat{\Lambda}|} \ln(\omega^2 - k^2) \right]. \quad (4.34)$$

Then

$$\tilde{F}(\eta) = F(\eta) - \frac{\pi}{|\hat{\Lambda}|} \int_0^\infty d\omega \frac{e^{-\omega^2/4\eta}}{\omega^2 - k^2} = F(\eta) - \frac{\pi}{|\hat{\Lambda}|} \int_0^\infty dt \frac{e^{-t/4\eta}}{t - k^2}$$

$$= |\hat{\Gamma}| \sum_{\lambda\in\Lambda} \tilde{G}_k(\lambda) e^{-i\lambda\theta} + o(1) \quad \text{as } \eta \to \infty, \quad (4.35)$$

and hence

$$(2\pi)^{-2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\omega}} \frac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - 2\pi \ln \omega \right]$$

$$= (2\pi)^{-2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma \\ |\gamma+\theta|\le\omega}} \frac{|\hat{\Lambda}|}{|\gamma+\theta|^2 - k^2} - \pi \ln(\omega^2 - k^2) \right]$$

$$= |\hat{\Gamma}|^{-1} \lim_{\omega\to\infty} \left[f(\omega) - \frac{\pi}{|\hat{\Lambda}|} \ln(\omega^2 - k^2) \right]$$

$$= |\hat{\Gamma}|^{-1} \lim_{\eta\to\infty} \tilde{F}(\eta) + \frac{1}{2\pi} \ln(k/i)$$

$$= \sum_{\lambda\in\Lambda} \tilde{G}_k(\lambda) e^{-i\lambda\theta} + \frac{1}{2\pi} \ln(k/i). \quad (4.36)$$

■

Theorems 4.1 and 4.3 give rise to two self-adjoint operators, namely $-\hat{\Delta}_{\alpha,\Lambda}$ and $\int_{\hat{\Lambda}}^{\oplus} d^2\theta\, [-\hat{\Delta}_{\alpha,\Lambda}(\theta)]$, respectively, which are expected to be unitarily equivalent. However, since they are obtained via different nontrivial limit procedures, this has to be verified.

Theorem 4.5. *Define $\mathscr{U}$ to be the unitary operator*

$$\begin{aligned} &\mathscr{U}: L^2(\mathbb{R}^2) \to L^2(\hat{\Lambda}, l^2(\Gamma)) \equiv \int_{\hat{\Lambda}}^{\oplus} d^2\theta\, l^2(\Gamma), \\ &(\mathscr{U}\hat{f})(\theta, \gamma) = \hat{f}(\gamma + \theta), \qquad \gamma \in \Gamma, \quad \theta \in \hat{\Lambda}, \quad \hat{f} \in L^2(\mathbb{R}^2). \end{aligned} \tag{4.37}$$

Let $\alpha \in \mathbb{R}$. Then

$$\mathscr{U}[-\hat{\Delta}_{\alpha,\Lambda}]\mathscr{U}^{-1} = \int_{\hat{\Lambda}}^{\oplus} d^2\theta\, [-\hat{\Delta}_{\alpha,\Lambda}(\theta)], \tag{4.38}$$

where $-\hat{\Delta}_{\alpha,\Lambda}$ and $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ are given by (4.10) *and* (4.25), *respectively.*

PROOF. Similar to that of Theorem 1.4.3. ∎

We will now compute the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}$. In order to analyze $\sigma(-\hat{\Delta}_{\alpha,\Lambda})$, we first study in detail the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$.

Theorem 4.6. *Let $\alpha \in \mathbb{R}$ and $\theta \in \hat{\Lambda}$. Then the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ is purely discrete, i.e.,*

$$\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda}(\theta)) = \varnothing, \qquad \theta \in \hat{\Lambda}, \tag{4.39}$$

and can be characterized as follows: Let

$$\mathbb{R} - |\Gamma + \theta|^2 = \bigcup_{n=0}^{\infty} I_n(\theta), \tag{4.40}$$

where $I_n(\theta)$, $n \in \mathbb{N}_0$, are open intervals, and $|\Gamma + \theta|^2$ is defined in analogy to (1.4.24). *In each interval $I_n(\theta)$, $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ has exactly one simple eigenvalue $E_n^{\alpha,\Lambda}(\theta) = [k_n^{\theta,\Lambda}(\theta)]^2$ with eigenfunction*

$$\psi_{E_n^{\alpha,\Lambda}(\theta)}(\theta, \gamma) = [|\gamma + \theta|^2 - E_n^{\alpha,\Lambda}(\theta)]^{-1}, \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma. \tag{4.41}$$

$E_n^{\alpha,\Lambda}(\theta)$ is the unique solution of

$$\begin{gathered} \alpha - \frac{1}{2\pi}\Psi(1) = g_{k_n^{\alpha,\Lambda}(\theta)}(\theta), \\ \operatorname{Im} k_n^{\alpha,\Lambda}(\theta) \geq 0, \quad E_n^{\alpha,\Lambda}(\theta) = [k_n^{\alpha,\Lambda}(\theta)]^2 \in I_n(\theta). \end{gathered} \tag{4.42}$$

$E_n^{\alpha,\Lambda}(\theta)$, $\theta \in \hat{\Lambda}$, $n \in \mathbb{N}$, is strictly increasing in $\alpha \in \mathbb{R}$. In addition, $E^{\Lambda}(\theta) \in |\Gamma + \theta|^2$ is an eigenvalue of $-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ of multiplicity $m \geq 1$ iff there exist $m + 1$ points $\gamma_0, \ldots, \gamma_m \in \Gamma$ such that

$$E^{\Lambda}(\theta) = |\gamma_0 + \theta|^2 = \cdots = |\gamma_m + \theta|^2. \tag{4.43}$$

The corresponding eigenspace is spanned by the eigenfunctions

$$\psi^{(j)}_{E^{\Lambda}(\theta)}(\gamma) = \delta_{\gamma\gamma_j} - \delta_{\gamma\gamma_0}, \qquad \theta \in \hat{\Lambda}, \quad \gamma \in \Gamma, \quad j = 1, \ldots, m. \tag{4.44}$$

$-\hat{\Delta}_{\alpha,\Lambda}(\theta)$ *has no other eigenvalues.*

PROOF. Similar to that of Theorem 1.4.4. ∎

Remark. The proof of Theorem 4.6 actually provides a natural numbering of the eigenvalues of $-\Delta_{\alpha,\Lambda}(\theta)$, cf. the remark after Theorem 1.4.4, p. 192.

Our next result is the computation of the spectrum of $-\hat{\Delta}_{\alpha,\Lambda}$.

Theorem 4.7. *Let Λ be a lattice in the sense of* (4.16) *and let $\alpha \in \mathbb{R}$. Then the spectrum of the operator $-\hat{\Delta}_{\alpha,\Lambda}$ is purely absolutely continuous and equals*

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda}) = \sigma_{\mathrm{ac}}(-\hat{\Delta}_{\alpha,\Lambda}) = [E_0^{\alpha,\Lambda}(0), E_0^{\alpha,\Lambda}(\theta_0)] \cup [E_1^{\alpha,\Lambda}, \infty),$$
$$\sigma_{\mathrm{sc}}(-\hat{\Delta}_{\alpha,\Lambda}) = \varnothing, \qquad \alpha \in \mathbb{R}, \tag{4.45}$$

where

$$\theta_0 = -\tfrac{1}{2}(b_1 + b_2) \tag{4.46}$$

and

$$E_1^{\alpha,\Lambda} = \min\{E_{b_-}^{\alpha,\Lambda}(0), \tfrac{1}{4}|b_-|^2\} = \min_{\theta \in \hat{\Lambda}} E_{b_-}^{\alpha,\Lambda}(\theta), \tag{4.47}$$

where $b_- \in \{b_1, \mathrm{b}_2\}$ is such that

$$|b_-| \le |b_j|, \qquad j = 1, 2. \tag{4.48}$$

We have that

$$E_1^{\alpha,\Lambda} > 0, \qquad \alpha \in \mathbb{R} \tag{4.49}$$

and

$$E_0^{\alpha,\Lambda}(\theta_0) < 0 \quad \text{iff} \quad \alpha \le \alpha_{0,\Lambda} \tag{4.50}$$

with

$$\alpha_{0,\Lambda} = g_0(\theta_0). \tag{4.51}$$

Furthermore, the spectrum is monotone increasing in α in the sense that

$$\frac{\partial E_\gamma^{\alpha,\Lambda}(\theta)}{\partial \alpha} > 0, \quad \gamma \in \Gamma, \quad \theta \in \hat{\Lambda}, \qquad \frac{\partial E_1^{\alpha,\Lambda}}{\partial \alpha} \ge 0. \tag{4.52}$$

In addition

$$E_0^{\alpha,\Lambda}(0) \to \begin{cases} 0, & \alpha \to \infty, \\ -\infty, & \alpha \to -\infty, \end{cases} \qquad E_0^{\alpha,\Lambda}(\theta_0) \to \begin{cases} |\theta_0|^2, & \alpha \to \infty, \\ -\infty, & \alpha \to -\infty, \end{cases}$$
$$E_1^{\alpha,\Lambda} \to \begin{cases} \tfrac{1}{4}|b_-|^2, & \alpha \to \infty, \\ 0, & \alpha \to -\infty, \end{cases} \tag{4.53}$$

and hence there exists an $\alpha_{1,\Lambda} \in \mathbb{R}$ *such that*

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda}) = [E_0^{\alpha,\Lambda}(0), \infty), \qquad \alpha \geq \alpha_{1,\Lambda}. \tag{4.54}$$

PROOF. Similar to that of Theorem 1.4.5 except for the fact that in three dimensions there are infinitely many $\tilde{\theta}$'s satisfying (1.4.120) (all lying on a line), while in two dimensions we can find exactly one $\tilde{\theta}$ such that (1.4.120) is fulfilled. ∎

The difference in the computation of $\sigma(-\hat{\Delta}_{\alpha,\Lambda})$ in two and three dimensions sheds some light one the *Bethe–Sommerfeld conjecture* [450]. This conjecture states that Schrödinger operators with periodic interactions have infinitely many gaps in their spectrum in one dimension, while they only have finitely many gaps in their spectrum in higher dimensions. We have now seen that the Schrödinger operator with periodic point interactions fulfills the Bethe–Sommerfeld conjecture. However, as we have observed it was more difficult to "close the gaps" in two dimensions than in three dimensions, and it is not possible at all in one dimension for the Kronig–Penney model. In this sense the periodic δ'-model of Ch. 3 also fulfills the Bethe–Sommerfeld conjecture since there are always infinitely many open gaps (although the first gap might close).

Finally, we discuss the infinite straight polymer in two dimensions, i.e., the analysis of $-\hat{\Delta}_{\alpha,\Lambda_1}$ where

$$\Lambda_1 = \{(0, na) \in \mathbb{R}^2 | n \in \mathbb{Z}\}, \qquad a > 0. \tag{4.55}$$

To decompose $-\hat{\Delta}_{\alpha,\Lambda_1}$ we introduce the unitary operators

$$\begin{gathered}\mathscr{U}_1\colon L^2(\mathbb{R}^2) \to L^2(\hat{\Lambda}_1, L^2(\mathbb{R} \times \Gamma_1)) = \int_{\hat{\Lambda}_1}^{\oplus} d\theta\, L^2(\mathbb{R} \times \Gamma_1), \\ (\mathscr{U}_1 \hat{f})(\theta, p, \gamma) = \hat{f}(p, \gamma + \theta), \qquad \theta \in \hat{\Lambda}_1, \quad \gamma \in \Gamma_1, \quad p \in \mathbb{R}, \quad \hat{f} \in L^2(\mathbb{R}^2),\end{gathered} \tag{4.56}$$

where

$$\hat{\Lambda}_1 = \left[-\frac{\pi}{a}, \frac{\pi}{a}\right), \qquad \Gamma_1 = \left\{\left(0, \frac{2\pi}{a} n\right) \in \mathbb{R}^2 | n \in \mathbb{Z}\right\}.$$

The fiber of the resolvent of the free Hamiltonian $-\hat{\Delta}$ with respect to the decomposition defined by (4.49) then reads

$$\begin{gathered}G_k(\theta)\colon L^2(\mathbb{R} \times \Gamma_1) \to L^2(\mathbb{R} \times \Gamma_1) \\ (G_k(\theta)g)(p, \gamma) = [|(p, \gamma + \theta)|^2 - k^2]^{-1} g(p, \gamma), \\ \theta \in \hat{\Lambda}_1, \quad k^2 \notin [\theta^2, \infty), \quad \operatorname{Im} k \geq 0.\end{gathered} \tag{4.57}$$

We can then state the following

Theorem 4.8. *Let* Λ_1 *be given by* (4.55). *Then we have*

$$\mathscr{U}_1[-\hat{\Delta}_{\alpha,\Lambda_1}]\mathscr{U}_1^{-1} = \int_{\hat{\Lambda}_1}^{\oplus} d\theta\, [-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)], \tag{4.58}$$

where $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ *is the self-adjoint operator in* $L^2(\mathbb{R} \times \Gamma_1)$ *with resolvent*

$$(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta) - k^2)^{-1}$$
$$= G_k(\theta) + \left\{\alpha - \frac{1}{2\pi}[\Psi(1) + \ln 2] - g_k(\theta)\right\}^{-1} (\overline{G_k(\theta)}, \cdot)G_k(\theta),$$
$$\theta \in \hat{\Lambda}_1, \quad k^2 \in \rho(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)), \quad \operatorname{Im} k \geq 0, \tag{4.59}$$

where

$$g_k(\theta) = (2\pi)^{-2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma_1 \\ |\gamma+\theta|\leq\omega}} \frac{a}{\sqrt{|\gamma + \theta|^2 - k^2}} - 2\pi \ln \omega \right], \qquad \operatorname{Im} k \geq 0. \tag{4.60}$$

Proof. Following the proof of Theorem 1.4.8 we find (4.59) with

$$g_k(\theta) = \sum_{\lambda\in\Lambda_1} \tilde{G}_k(\lambda)e^{-i\lambda\theta} - \frac{1}{2\pi}\ln(k/i), \qquad \operatorname{Im} k > 0. \tag{4.61}$$

Using the Poisson summation formula, Lemma 4.9, the result follows. ■

Lemma 4.9 (Poisson Summation Formula). *Let* $k^2 \in \mathbb{C}$, $\operatorname{Im} k > 0$, *and* $\theta \in \hat{\Lambda}_1$. *Then*

$$\sum_{\lambda\in\Lambda_1} \tilde{G}_k(\lambda)e^{-i\lambda\theta} = (2\pi)^{-2} \lim_{\omega\to\infty} \left[\sum_{\substack{\gamma\in\Gamma_1 \\ |\gamma+\theta|\leq\omega}} \frac{a}{\sqrt{|\gamma + \theta|^2 - k^2}} - 2\pi \ln \omega \right]. \tag{4.62}$$

Proof. Similar to that of Lemma 4.4. ■

From (4.59) we read off the spectral properties of $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$.

Theorem 4.10. *Let* $\alpha \in \mathbb{R}$, $\theta \in \hat{\Lambda}_1$. *Then the essential spectrum of* $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ *is purely absolutely continuous and equals*

$$\sigma_{\text{ess}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \sigma_{\text{ac}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = [\theta^2, \infty), \qquad \sigma_{\text{sc}}(-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)) = \varnothing. \tag{4.63}$$

In addition, $-\hat{\Delta}_{\alpha,\Lambda_1}(\theta)$ *has one simple eigenvalue* $E^{\alpha,\Lambda_1}(\theta) = [k^{\alpha,\Lambda_1}(\theta)]^2 < \theta^2$ *which is the unique solution of*

$$\alpha = \frac{1}{2\pi}[\Psi(1) + \ln 2] + g_{k^{\alpha,\Lambda_1}(\theta)}(\theta),$$
$$\operatorname{Im} k^{\alpha,\Lambda_1}(\theta) \geq 0, \quad \operatorname{Re} k^{\alpha,\Lambda_1}(\theta) \geq 0. \tag{4.64}$$

The corresponding eigenfunction reads

$$\psi_{E^{\alpha,\Lambda_1}(\theta)}(\theta, p, \gamma) = [|(p, \gamma + \theta)|^2 - E^{\alpha,\Lambda_1}(\theta)]^{-1}, \qquad \theta \in \hat{\Lambda}_1, \quad p \in \mathbb{R}, \quad \gamma \in \Gamma_1. \tag{4.65}$$

$E^{\alpha,\Lambda_1}(\theta)$, $\theta \in \hat{\Lambda}_1$, *is strictly increasing in* $\alpha \in \mathbb{R}$.

PROOF. Similar to that of Theorem 1.6.3. ■

As the final result in this chapter we compute the spectrum of $-\hat{\Delta}_{\alpha,\Lambda_1}$.

Theorem 4.11. *Let $\alpha \in \mathbb{R}$ and Λ_1 be given by* (4.55) *Then the spectrum of* $-\hat{\Delta}_{\alpha,\Lambda_1}$ *is purely absolutely continuous and equals*

$$\sigma(-\hat{\Delta}_{\alpha,\Lambda_1}) = \sigma_{\mathrm{ac}}(-\hat{\Delta}_{\alpha,\Lambda_1}) = \begin{cases} [E^{\alpha,\Lambda_1}(0), \infty), & \alpha \geq \alpha_{\Lambda_1}, \\ [E^{\alpha,\Lambda_1}(0), E^{\alpha,\Lambda_1}(-\pi/a)] \cup [0, \infty), & \alpha < \alpha_{\Lambda_1}, \end{cases} \tag{4.66}$$

with $E^{\alpha,\Lambda_1}(0) < 0$, $\alpha \in \mathbb{R}$, *and* $E^{\alpha,\Lambda_1}(0) < E^{\alpha,\Lambda_1}(-\pi/a) < 0$ *provided* $\alpha < \alpha_{\Lambda_1}$ *where* α_{Λ_1} *equals*

$$\alpha_{\Lambda_1} = \frac{1}{2\pi}[\Psi(1) + \ln 2] + (2\pi)^{-2} \lim_{\omega \to \infty} \left[\sum_{\substack{\gamma \in \Gamma_1 \\ |\gamma - \frac{\pi}{a}| \leq \omega}} \frac{a}{\left|\gamma - \dfrac{\pi}{a}\right|} - 2\pi \ln \omega \right]. \tag{4.67}$$

Furthermore, the spectrum of $-\hat{\Delta}_{\alpha,\Lambda_1}$ *is monotone increasing in* $\alpha \in \mathbb{R}$ *in the sense that*

$$\frac{\partial E^{\alpha,\Lambda_1}(\theta)}{\partial \alpha} > 0, \qquad \theta \in \hat{\Lambda}_1. \tag{4.68}$$

PROOF. Similar to that of Theorem 1.4.5. ■

Notes

The presentation is taken from Albeverio, Gesztesy, Høegh-Krohn, and Holden [19]. The discussion of the infinite straight polymer can partly be found in [227]. The Bethe–Sommerfeld conjecture has been proved for a general class of potentials in two and three dimensions by Skriganov [442], [443], [444], a generalization in two dimensions also appeared in [130].

The two-dimensional crystal in a homogeneous magnetic field has been studied in [196].

CHAPTER III.5

Random Hamiltonians with Point Interactions

III.5.1 Preliminaries

In this section we recall general properties of the spectrum of ergodic random Hamiltonians.

Let $(\Omega, \mathscr{F}, P)$ be a complete probability space. Furthermore, let $\mathscr{H}$ be a separable, complex Hilbert space and let $\{H_\omega\}_{\omega \in \Omega}$ be a family of P-a.s. self-adjoint operators in $\mathscr{H}$. The family $\{H_\omega\}_{\omega \in \Omega}$ is called *measurable* iff $\omega \to (H_\omega - z)^{-1}$ is weakly measurable for all $z \in \mathbb{C} - \mathbb{R}$, i.e., iff

$$\omega \to (\phi, (H_\omega - z)^{-1}\psi), \qquad \phi, \psi \in \mathscr{H}, \quad z \in \mathbb{C} - \mathbb{R}, \tag{5.1.1}$$

is measurable. Quite generally, we call a family of bounded operators $\{A_\omega\}_{\omega \in \Omega}$ *weakly measurable* iff $\omega \to (\phi, A_\omega \psi)$, ϕ, $\psi \in \mathscr{H}$ is measurable. It is straightforward to prove that $\omega \to (H_\omega - z)^{-1}$ is weakly measurable for all $z \in \mathbb{C} - \mathbb{R}$ if $\omega \to (H_\omega - z_0)^{-1}$ is weakly measurable for some $z_0 \in \mathbb{C}$ and for P-a.e. $\omega \in \Omega$ the distance $d(z_0, \sigma(H_\omega)) \geq \varepsilon$ (independent of ω). We start with

Lemma 5.1.1. *Let $\{H_\omega\}_{\omega \in \Omega}$ be a family of P-a.s. self-adjoint operators in $\mathscr{H}$. Then the following assertions* (i)–(iv) are equivalent.

(i) $\omega \to (H_\omega - z)^{-1}$ *is weakly measurable for all* $z \in \mathbb{C} - \mathbb{R}$.
(ii) $\omega \to E_\omega(\lambda)$ *(the spectral projections associated with* H_ω*) is weakly measurable for all* $\lambda \in \mathbb{R}$.
(iii) $\omega \to e^{itH_\omega}$ *is weakly measurable for all* $t \in \mathbb{R}$.
(iv) $\omega \to f(H_\omega)$ *is weakly measurable for any bounded, measurable function* $f\colon \mathbb{R} \to \mathbb{R}$.

PROOF. It suffices to recall that

$$(\phi, e^{itH_\omega}\psi) = \int_{\mathbb{R}} d(\phi, E_\omega(\lambda)\psi)e^{it\lambda}, \qquad t \in \mathbb{R}, \tag{5.1.2}$$

$$(\phi, (H_\omega - z)^{-1}\psi) = \pm \int_0^\infty dt\, e^{\pm izt}(\phi, e^{\mp itH_\omega}\psi), \qquad \operatorname{Im} z \gtrless 0, \tag{5.1.3}$$

$$(\phi, E_\omega(\lambda)\psi)$$
$$= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} (2\pi i)^{-1} \int_{-\infty}^{\lambda+\delta} dt(\phi, [(H_\omega - t - i\varepsilon)^{-1} - (H_\omega - t + i\varepsilon)^{-1}]\psi),$$
$$\lambda \in \mathbb{R}; \quad \phi, \psi \in \mathscr{H}, \tag{5.1.4}$$

and the fact that $f_\pm = (|f| \pm f)/2$ is a uniform limit of appropriate step functions $f_{n(\pm)}$ with $0 \le f_{n(\pm)} \le f_\pm$. ■

Remark. Here $\omega \to (\phi, (H_\omega - z)^{-1}\psi)$, $\omega \to (\phi, E_\omega(\lambda)\psi)$, etc. are only defined in the complement of a set of P-measure zero. On this set we may simply define these functions to be zero. This convention will always be used from now on.

Lemma 5.1.2.

(i) *Assume that $\omega \to A_\omega$, $\omega \to B_\omega$ are weakly measurable, bounded operators in $\mathscr{H}$. Then $\omega \to A_\omega B_\omega$ is also weakly measurable.*
(ii) *Assume the family $\{H_\omega\}_{\omega \in \Omega}$ of bounded, P-a.s. self-adjoint operators in $\mathscr{H}$ to be weakly measurable. Then the family $\{H_\omega\}_{\omega \in \Omega}$ is in fact measurable in the sense defined in* (5.1.1).

PROOF. Let $\{\phi_n\}_{n \in \mathbb{N}}$ be an orthonormal basis in $\mathscr{H}$. Then

$$(\phi, A_\omega B_\omega \psi) = \sum_{n \in \mathbb{N}} (\phi, A_\omega \phi_n)(\phi_n, B_\omega \psi), \qquad \phi, \psi \in \mathscr{H}, \tag{5.1.5}$$

proves (i).

In order to prove part (ii), we note that (i) implies that $\{H_\omega^m\}_{\omega \in \Omega}$, $m \in \mathbb{N}$, and hence polynomials

$$\{P(H_\omega)\}_{\omega \in \Omega}, \qquad P(x) = \sum_{m=0}^{M} a_m x^m, \qquad a_m \in \mathbb{C}, \quad m = 1, \ldots, M, \quad x \in \mathbb{R}, \tag{5.1.6}$$

are weakly measurable. Applying the Stone–Weierstrass approximation argument, we infer that for bounded, continuous functions $f\colon \mathbb{R} \to \mathbb{C}$, $\{f(H_\omega)\}_{\omega \in \Omega}$ is weakly measurable. In particular, by choosing $f(x) = e^{itx}$, $t \in \mathbb{R}$, we see that (ii) follows using Lemma 5.1.1(iii). ■

Another useful result for the final applications we have in mind is

Lemma 5.1.3. *For each $n \in \mathbb{N}$, let $\{H_\omega^{(n)}\}_{\omega \in \Omega}$ be a family of P-a.s. self-adjoint operators in $\mathscr{H}$ which is measurable. Assume that for P-a.e. $\omega \in \Omega$, $H_\omega^{(n)}$ converges in weak (and hence also in strong) resolvent sense to a self-adjoint operator H_ω in $\mathscr{H}$. Then the family $\{H_\omega\}_{\omega \in \Omega}$ is measurable.*

PROOF. Since P-a.e. limits of measurable functions are again measurable, the result follows from

$$(\phi, (H_\omega^{(n)} - z)^{-1}\psi) \xrightarrow[n\to\infty]{P\text{-a.s.}} (\phi, (H_\omega - z)^{-1}\psi), \qquad \phi, \psi \in \mathscr{H}, \quad z \in \mathbb{C} - \mathbb{R}. \quad (5.1.7)$$

■

Without further assumptions, the various types of spectra associated with H_ω in general will strongly depend on ω. In order to get spectra which are nonrandom sets we introduce the notion of ergodicity: Let I be some index set and suppose that $\{T_j\}_{j\in I}$ is a family of measure preserving, *ergodic transformations* on $(\Omega, \mathscr{F}, P)$ in the sense that

$$P(T_j^{-1}B) = P(B), \qquad B \in \mathscr{F}, \quad j \in I, \tag{5.1.8}$$

and that

$$A \in \mathscr{F}, \qquad T_j^{-1}A = A, \qquad j \in I \quad \text{implies} \quad P(A) = 0 \quad \text{or} \quad P(A) = 1. \tag{5.1.9}$$

In addition, we assume the existence of unitary operators U_j, $j \in I$, in $\mathscr{H}$ which are related to $T_j, j \in I$, by the equation

$$U_j H_\omega U_j^{-1} = H_{T_j\omega}, \qquad j \in I. \tag{5.1.10}$$

If these assumptions are satisfied and if $\{H_\omega\}_{\omega\in\Omega}$ is measurable, we call $\{H_\omega\}_{\omega\in\Omega}$ an *ergodic family* of P-a.s. self-adjoint operators in $\mathscr{H}$.

We state

Lemma 5.1.4. *Let $\{H_\omega\}_{\omega\in\Omega}$ be an ergodic family of P-a.s. self-adjoint operators in $\mathscr{H}$ and let $\{E_\omega(\lambda)\}_{\omega\in\Omega}$, $\lambda \in \mathbb{R}$, be the corresponding spectral projections. Then there is a subset $\Omega_0 \subseteq \Omega$ with $P(\Omega_0) = 1$ such that for all $\omega \in \Omega_0$ and all $\lambda, \mu \in \mathbb{Q}$, $\lambda \geq \mu$, $\dim\{\mathrm{Ran}[E_\omega(\lambda) - E_\omega(\mu)]\}$ equals a constant $C_{\lambda,\mu}$ (possibly infinite) on Ω_0.*

PROOF. Denote by

$$f_{\lambda,\mu}(\omega) = \dim\{\mathrm{Ran}[E_\omega(\lambda) - E_\omega(\mu)]\} = \mathrm{Tr}[E_\omega(\lambda) - E_\omega(\mu)],$$
$$\lambda, \mu \in \mathbb{R}, \quad \lambda \geq \mu, \quad \omega \in \Omega, \tag{5.1.11}$$

where $\mathrm{Tr}(\cdot)$ abbreviates the trace. Clearly,

$$f_{\lambda,\mu}(T_j\omega) = f_{\lambda,\mu}(\omega), \qquad j \in I, \tag{5.1.12}$$

since (5.1.10) implies

$$U_j E_\omega(\lambda) U_j^{-1} = E_{T_j\omega}(\lambda), \qquad \lambda \in \mathbb{R}, \quad j \in I. \tag{5.1.13}$$

Moreover, $f_{\lambda,\mu}$ is measurable since

$$f_{\lambda,\mu}(\omega) = \sum_{n\in\mathbb{N}} (\phi_n, [E_\omega(\lambda) - E_\omega(\mu)]\phi_n), \tag{5.1.14}$$

where $\{\phi_n\}_{n\in\mathbb{N}}$ is any orthonormal basis in $\mathscr{H}$, because $\omega \to (\phi_n, E_\omega(\lambda)\phi_n)$, $\lambda \in \mathbb{R}$, is measurable by assumption. Since $\{T_j\}_{j\in I}$ is ergodic, (5.1.12) implies that $f_{\lambda,\mu}$ is P-a.s. constant (cf., e.g., [388], Sect. II.5). Thus there exists a subset $\Omega_{\lambda,\mu} \subset \Omega$ with

$P(\Omega_{\lambda,\mu}) = 1$ such that $f_{\lambda,\mu}(\omega) = C_{\lambda,\mu}$ for all $\omega \in \Omega_{\lambda,\mu}$. Introducing $\Omega_0 = \bigcap_{\lambda,\mu \in \mathbb{Q}} \Omega_{\lambda,\mu}$ we finally get

$$P(\Omega_0) = 1, \qquad f_{\lambda,\mu}(\omega) = C_{\lambda,\mu}, \qquad \omega \in \Omega_0, \quad \lambda, \mu \in \mathbb{Q}. \tag{5.1.15}$$

∎

Given Lemma 5.1.4 we are able to formulate the first main result

Theorem 5.1.5. *Let $\{H_\omega\}_{\omega \in \Omega}$ be an ergodic family of P-a.s. self-adjoint operators in $\mathscr{H}$. Then there are sets Σ, Σ_{ess}, $\Sigma_d \subseteq \mathbb{R}$ such that*

$$\sigma(H_\omega) = \Sigma, \tag{5.1.16}$$

$$\sigma_{\text{ess}}(H_\omega) = \Sigma_{\text{ess}}, \tag{5.1.17}$$

$$\sigma_{\text{d}}(H_\omega) = \Sigma_{\text{d}}, \tag{5.1.18}$$

*for P-*a.e. $\omega \in \Omega$. (*Here* $\sigma_{\text{d}}(\cdot) = \sigma(\cdot) - \sigma_{\text{ess}}(\cdot)$ *denotes the discrete spectrum.*)

PROOF. Using the strong right continuity of spectral projections we have

$$\begin{aligned}
\lambda \in \sigma(H_\omega) &\Leftrightarrow \forall \varepsilon > 0\colon E_\omega(\lambda + \varepsilon) - E_\omega(\lambda - \varepsilon) \neq 0 \\
&\Leftrightarrow \forall \lambda', \lambda'' \in \mathbb{Q}, \qquad \lambda'' < \lambda < \lambda'\colon E_\omega(\lambda') - E_\omega(\lambda'') \neq 0 \\
&\Leftrightarrow \forall \lambda', \lambda'' \in \mathbb{Q}, \qquad \lambda'' < \lambda < \lambda'\colon f_{\lambda',\lambda''}(\omega) \neq 0.
\end{aligned} \tag{5.1.19}$$

But $f_{\lambda',\lambda''}$ is P-a.s. constant by Lemma 5.1.4. Hence $\lambda \in \sigma(H_\omega)$ is P-a.s. independent of $\omega \in \Omega$. Similarly, we obtain

$$\begin{aligned}
\lambda \in \sigma_{\text{ess}}(H_\omega) &\Leftrightarrow \forall \varepsilon > 0\colon \dim\{\operatorname{Ran}[E_\omega(\lambda + \varepsilon) - E_\omega(\lambda - \varepsilon)]\} = \infty \\
&\Leftrightarrow \forall \lambda', \lambda'' \in \mathbb{Q}, \qquad \lambda'' < \lambda < \lambda'\colon f_{\lambda',\lambda''}(\omega) = \infty.
\end{aligned} \tag{5.1.20}$$

Hence, again by Lemma 5.1.4, $\lambda \in \sigma_{\text{ess}}(H_\omega)$ is P-a.s. independent of $\omega \in \Omega$. Since $\sigma_{\text{d}}(H_\omega) = \sigma(H_\omega) - \sigma_{\text{ess}}(H_\omega)$, (5.1.18) follows from the above. ∎

In order to extend this result to the continuous, absolutely continuous, and singularly continuous spectrum of H_ω, we need the concept of analytic sets as introduced, e.g., in [341], Ch. III. For a proof of the following result see, e.g., [286], [287], [341].

Lemma 5.1.6.

(i) *Let $\mathscr{E}$ be a complete, separable metric space, $(\Omega, \mathscr{F})$ a measurable space, and let $\mathscr{A}(\mathscr{F})$ (resp. $\mathscr{A}(\mathscr{B}(\mathscr{E}) \times \mathscr{F})$) denote the $\mathscr{F}$- (resp. $\mathscr{B}(\mathscr{E}) \times \mathscr{F}$-) analytic sets in Ω (resp. $\mathscr{E} \times \Omega$) where $\mathscr{B}(\mathscr{E})$ denotes the Borel σ-algebra of $\mathscr{E}$. Then for $A \in \mathscr{A}(\mathscr{B}(\mathscr{E}) \times \mathscr{F})$ we have*

$$\operatorname{pr}_\Omega(A) = \{\omega \in \Omega \mid \exists x \in \mathscr{E}\colon (x, \omega) \in A\} \in \mathscr{A}(\mathscr{F}). \tag{5.1.21}$$

(ii) *If $(\Omega, \mathscr{F}, P)$ is a complete probability space, then $\mathscr{A}(\mathscr{F}) = \mathscr{F}$.*

(iii) *Assume, in addition, that $\mathscr{E}$ is a complex Hilbert space and $\mathscr{E}_\omega$ is a closed subspace of $\mathscr{E}$. Suppose that $\{(\phi, \omega) \in \mathscr{E} \times \Omega \mid \phi \in \mathscr{E}_\omega\}$ is $\mathscr{B}(\mathscr{E}) \times \mathscr{F}$ analytic. Then $P_{\mathscr{E}_\omega}$, the projection onto $\mathscr{E}_\omega$, is weakly measurable.*

Remark. One can show under the hypotheses of Lemma 5.1.6(i) that $\mathscr{F} \subseteq \mathscr{A}(\mathscr{F})$ and also $\mathscr{B}(\mathscr{E}) \otimes \mathscr{F} \subseteq \mathscr{A}(\mathscr{B}(\mathscr{E}) \times \mathscr{F})$ [341] where $\mathscr{B}(\mathscr{E}) \otimes \mathscr{F}$ denotes the σ-algebra generated by $\mathscr{B}(\mathscr{E}) \times \mathscr{F}$. Hence, in order to satisfy the hypotheses of Lemma 5.1.6(iii), we only need to show that $\{\phi, \omega) \in \mathscr{E} \times \Omega | \phi \in \mathscr{E}_\omega\}$ is measurable in the sense that it belongs to $\mathscr{B}(\mathscr{E}) \otimes \mathscr{F}$.

Lemma 5.1.6 implies

Lemma 5.1.7. *Let $\{H_\omega\}_{\omega \in \Omega}$ be a measurable family of P-a.s. self-adjoint operators in $\mathscr{H}$. Moreover, denote by P_ω^{c}, P_ω^{ac}, P_ω^{sc}, P_ω^{pp} the projections onto the continuous, absolutely continuous, singularly continuous, and pure point spectral subspace associated with H_ω. Then $\{P_\omega^{c}\}_{\omega \in \Omega}$, $\{P_\omega^{ac}\}_{\omega \in \Omega}$, $\{P_\omega^{sc}\}_{\omega \in \Omega}$, and $\{P_\omega^{pp}\}_{\omega \in \Omega}$ are weakly measurable.*

PROOF. Since a bounded, continuous and monotone function on $\mathbb{R}$ is uniformly continuous and spectral projections are strongly right continuous we get

$$\begin{aligned}
&\{(\phi, \omega) \in \mathscr{H} \times \Omega | \phi \in P_\omega^{c}\mathscr{H}\} \\
&\qquad = \{(\phi, \omega) \in \mathscr{H} \times \Omega | \lambda \to (\phi, E_\omega(\lambda)\phi) \text{ is continuous on } \mathbb{R}\} \\
&\qquad = \{(\phi, \omega) \in \mathscr{H} \times \Omega | \forall m \in \mathbb{N}, \exists n \in \mathbb{N}, \text{ s.t. } \forall \lambda, \lambda' \in \mathbb{R}: \\
&\qquad\qquad |\lambda - \lambda'| < n^{-1} \Rightarrow |(\phi, [E_\omega(\lambda) - E_\omega(\lambda')]\phi)| < m^{-1}\} \\
&\qquad = \{(\phi, \omega) \in \mathscr{H} \times \Omega | \forall m \in \mathbb{N}, \exists n \in \mathbb{N}, \text{ s.t. } \forall \lambda, \lambda' \in \mathbb{Q}: \\
&\qquad\qquad |\lambda - \lambda'| < n^{-1} \Rightarrow |(\phi, [E_\omega(\lambda) - E_\omega(\lambda')]\phi)| < m^{-1}\} \\
&\qquad = \bigcap_{m \in \mathbb{N}} \bigcup_{n \in \mathbb{N}} \bigcap_{\substack{\lambda, \lambda' \in \mathbb{Q} \\ |\lambda - \lambda'| < n^{-1}}} \{(\phi, \omega) \in \mathscr{H} \times \Omega || (\phi, [E_\omega(\lambda) - E_\omega(\lambda')]\phi)| < m^{-1}\}.
\end{aligned} \tag{5.1.22}$$

Since $\{H_\omega\}_{\omega \in \Omega}$ is measurable, the function $f(\phi, \omega) = (\phi, [E_\omega(\lambda) - E_\omega(\lambda')]\phi)$ is measurable for fixed $\phi \in \mathscr{H}$, $\lambda, \lambda' \in \mathbb{R}$. Moreover, f is continuous with respect to $\phi \in \mathscr{H}$ and hence f is (simultaneously) measurable with respect to $(\phi, \omega) \in \mathscr{H} \times \Omega$. Consequently, the set

$$\{(\phi, \omega) \in \mathscr{H} \times \Omega || (\phi, [E_\omega(\lambda) - E_\omega(\lambda')]\phi)| < m^{-1}\} \tag{5.1.23}$$

and hence also the set

$$\{(\phi, \omega) \in \mathscr{H} \times \Omega | \phi \in P_\omega^{c}\mathscr{H}\} \tag{5.1.24}$$

is $\mathscr{B}(\mathscr{H}) \otimes \mathscr{F}$ measurable. Now we only need to apply Lemma 5.1.6(iii) and the remark following it in order to infer the weak measurability of $\{P_\omega^{c}\}_{\omega \in \Omega}$. Next we note that

$$\begin{aligned}
&\{(\phi, \omega) \in \mathscr{H} \times \Omega | \phi \in P_\omega^{ac}\mathscr{H}\} \\
&\qquad = \left\{(\phi, \omega) \in \mathscr{H} \times \Omega | \exists g \in L^1(\mathscr{R}), \text{ s.t. } \forall \lambda \in \mathbb{R}: (\phi, E_\omega(\lambda)\phi) = \int_{-\infty}^{\lambda} dt\, g(t)\right\} \\
&\qquad = \left\{(\phi, \omega) \in \mathscr{H} \times \Omega | \exists g \in L^1(\mathbb{R}), \text{ s.t. } \forall \lambda \in \mathbb{Q}: (\phi, E_\omega(\lambda)\phi) = \int_{-\infty}^{\lambda} dt\, g(t)\right\}
\end{aligned}$$

$$= \mathrm{pr}_{\mathscr{H}\times\Omega}\left(\left\{(g, \phi, \omega) \in L^1(\mathbb{R}) \times \mathscr{H} \times \Omega \,|\, \forall \lambda \in \mathbb{Q}: (\phi, E_\omega(\lambda)\phi) = \int_{-\infty}^{\lambda} dt\, g(t)\right\}\right)$$

$$= \mathrm{pr}_{\mathscr{H}\times\Omega}\left(\bigcap_{\lambda\in\mathbb{Q}} \left\{(g, \phi, \omega) \in L^1(\mathbb{R}) \times \mathscr{H} \times \Omega \,|\, (\phi, E_\omega(\lambda)\phi) = \int_{-\infty}^{\lambda} dt\, g(t)\right\}\right). \tag{5.1.25}$$

The function $f(g, \phi, \omega) = (\phi, E_\omega(\lambda)\phi) - \int_{-\infty}^{\lambda} dt\, g(t)$ is measurable in ω and continuous in (g, ϕ). Hence the set

$$\{(g, \phi, \omega) \in L^1(\mathbb{R}) \times \mathscr{H} \times \Omega \,|\, f(g, \phi, \omega) = 0\} \tag{5.1.26}$$

is $\mathscr{B}(L^1(\mathbb{R})) \otimes \mathscr{B}(\mathscr{H}) \otimes \mathscr{F}$ measurable and thus analytic. Consequently, $\{(\phi, \omega) \in \mathscr{H} \times \Omega \,|\, \phi \in P_\omega^{\mathrm{ac}}\mathscr{H}\}$ is $\mathscr{B}(\mathscr{H}) \otimes \mathscr{F}$ analytic by Lemma 5.1.6(i). Lemma 5.1.6(ii) then proves that $\{P_\omega^{\mathrm{ac}}\}_{\omega\in\Omega}$ is weakly measurable. Since $P_\omega^{\mathrm{pp}} = 1 - P_\omega^{\mathrm{c}}$ and $P_\omega^{\mathrm{sc}} = P_\omega^{\mathrm{c}} - P_\omega^{\mathrm{ac}}$, the proof is complete. ∎

For an alternative approach to Lemma 5.1.7, cf. [119], [128].

Now we are able to extend Theorem 5.1.5 and state

Theorem 5.1.8. *Let $\{H_\omega\}_{\omega\in\Omega}$ be an ergodic family of P-a.s. self-adjoint operators in $\mathscr{H}$. Then there are sets $\Sigma_{\mathrm{c}}, \Sigma_{\mathrm{ac}}, \Sigma_{\mathrm{sc}}, \Sigma_{\mathrm{p}} \subseteq \mathbb{R}$ such that*

$$\sigma_{\mathrm{c}}(H_\omega) = \Sigma_{\mathrm{c}}, \tag{5.1.27}$$

$$\sigma_{\mathrm{ac}}(H_\omega) = \Sigma_{\mathrm{ac}}, \tag{5.1.28}$$

$$\sigma_{\mathrm{sc}}(H_\omega) = \Sigma_{\mathrm{sc}}, \tag{5.1.29}$$

$$\overline{\sigma_{\mathrm{p}}(H_\omega)} = \Sigma_{\mathrm{p}}, \tag{5.1.30}$$

for P-a.e. $\omega \in \Omega$.

PROOF. Define in analogy to (5.1.11)

$$\begin{aligned} f_{\lambda,\mu}^{\mathrm{c}}(\omega) &= \mathrm{Tr}[E_\omega^{\mathrm{c}}(\lambda) - E_\omega^{\mathrm{c}}(\mu)], \\ f_{\lambda,\mu}^{\mathrm{ac}}(\omega) &= \mathrm{Tr}[E_\omega^{\mathrm{ac}}(\lambda) - E_\omega^{\mathrm{ac}}(\mu)], \qquad \lambda, \mu \in \mathbb{R}, \quad \lambda \geq \mu, \quad \omega \in \Omega, \end{aligned} \tag{5.1.31}$$

where

$$E_\omega^{\mathrm{c}}(\lambda) = E_\omega(\lambda)P_\omega^{\mathrm{c}}, \qquad E_\omega^{\mathrm{ac}}(\lambda) = E_\omega(\lambda)P_\omega^{\mathrm{ac}}, \qquad \lambda \in \mathbb{R}, \quad \omega \in \Omega. \tag{5.1.32}$$

By Lemma 5.1.2(i), $\{E_\omega^{\mathrm{c}}(\lambda)\}_{\omega\in\Omega}$ and $\{E_\omega^{\mathrm{ac}}(\lambda)\}_{\omega\in\Omega}$, $\lambda \in \mathbb{R}$, are measurable, implying measurability of $f_{\lambda,\mu}^{\mathrm{c}}$ and $f_{\lambda,\mu}^{\mathrm{ac}}$. Moreover, (5.1.10) implies

$$U_j P_\omega^{\mathrm{c}} U_j^{-1} = P_{T_j\omega}^{\mathrm{c}}, \qquad U_j P_\omega^{\mathrm{ac}} U_j^{-1} = P_{T_j\omega}^{\mathrm{ac}}, \qquad j \in I, \tag{5.1.33}$$

and hence

$$f_{\lambda,\mu}^{\mathrm{c}}(T_j\omega) = f_{\lambda,\mu}^{\mathrm{c}}(\omega), \qquad f_{\lambda,\mu}^{\mathrm{ac}}(T_j\omega) = f_{\lambda,\mu}^{\mathrm{ac}}(\omega), \qquad j \in I. \tag{5.1.34}$$

Since $\{T_j\}_{j\in I}$ is ergodic, we can follow the last part in the proof of Lemma 5.1.4 and the proof of (5.1.16) to infer that $H_\omega P_\omega^{\mathrm{c}}$ and $H_\omega P_\omega^{\mathrm{ac}}$ have P-a.s. constant spectrum. The fact that $\sigma_{\mathrm{p}}(H_\omega) = \sigma(H_\omega[1 - P_\omega^{\mathrm{c}}])$ and $\sigma_{\mathrm{sc}}(H_\omega) = \sigma_{\mathrm{c}}(H_\omega[P_\omega^{\mathrm{c}} - P_\omega^{\mathrm{ac}}])$ then completes the proof. ∎

Finally, we study the discrete spectrum in more detail. Let $\{U_j\}_{j\in I}$ be a family of unitary operators in $\mathscr{H}$. We call $\{U_j\}_{j\in I}$ *complete* iff there exists an infinite subset $I_0 \subseteq I$ such that

$$\mathscr{A}_{I_0} = \{\phi \in \mathscr{H} | (U_j^*\phi, U_{j'}^*\phi) = 0, j \neq j', j, j' \in I_0\} \tag{5.1.35}$$

is total in $\mathscr{H}$. Since $\mathscr{H}$ is separable, I_0 is necessarily countable.

We have

Lemma 5.1.9. *Let $\{P_\omega\}_{\omega\in\Omega}$ be an ergodic family of (orthogonal) projections in $\mathscr{H}$ and assume the associated family of unitary operators $\{U_j\}_{j\in I}$ to be complete. Then either* $\dim[\mathrm{Ran}(P_\omega)] = 0$ *P-a.s. or* $\dim[\mathrm{Ran}(P_\omega)] = \infty$ *P-a.s.*

PROOF. Since $\mathrm{Tr}(P_\omega)$ is measurable and invariant under $\{T_j\}_{j\in I}$, $\dim[\mathrm{Ran}(P_\omega)] = \mathrm{Tr}(P_\omega)$ is P-a.s. constant. Hence

$$\mathrm{Tr}(P_\omega) = E(\mathrm{Tr}(P_\omega)) \quad P\text{-a.s.}, \tag{5.1.36}$$

where $E(\cdot)$ denotes expectation with respect to P. Let $\mathrm{I}_0 = \{j_n\}_{n\in\mathbb{N}}$ be such that

$$\mathscr{A}_{I_0} = \{\phi \in \mathscr{H} | (U_{j_n}^*\phi, U_{j_m}^*\phi) = 0, n \neq m, n, m \in \mathbb{N}\} \tag{5.1.37}$$

is total in $\mathscr{H}$. Choose $\phi \in \mathscr{A}_{I_0}$ with $\|\phi\| = 1$. Then $\{\phi_n = U_{j_n}^*\phi\}_{n\in\mathbb{N}}$ is an orthonormal basis in $\mathscr{H}$. Hence

$$\mathrm{Tr}(P_\omega) \geq \sum_{n=1}^{N} (\phi_n, P_\omega\phi_n), \qquad N \in \mathbb{N}, \tag{5.1.38}$$

and thus

$$\mathrm{Tr}(P_\omega) = E(\mathrm{Tr}(P_\omega)) \geq \sum_{n=1}^{\infty} E((\phi_n, P_\omega\phi_n)) \quad P\text{-a.s.} \tag{5.1.39}$$

Since T_j, $j \in I$, are measure preserving we infer

$$\begin{aligned} E((\phi_n, P_\omega\phi_n)) &= E((\phi, U_{j_n}P_\omega U_{j_n}^{-1}\phi)) \\ &= E((\phi, P_{T_{j_n}\omega}\phi)) = E((\phi, P_\omega\phi)), \qquad n \in \mathbb{N}. \end{aligned} \tag{5.1.40}$$

Hence either $E((\phi, P_\omega\phi)) = 0$ for all $\phi \in \mathscr{A}_{I_0}$ or $\mathrm{Tr}(P_\omega) = \infty$ P-a.s. In the first case we conclude that $(\phi, P_\omega\phi) = 0$ P-a.s. for all $\phi \in \mathscr{A}_{I_0}$. Since $\mathscr{A}_{I_0}$ is total in $\mathscr{H}$ we finally get $P_\omega = 0$ P-a.s. ∎

Thus we obtain

Theorem 5.1.10. *Let $\{H_\omega\}_{\omega\in\Omega}$ be an ergodic family of P-a.s. self-adjoint operators in $\mathscr{H}$ and assume the associated unitary family $\{U_j\}_{j\in I}$ to be complete. Then*

$$\Sigma_{\mathrm{d}} = \varnothing, \tag{5.1.41}$$

i.e., $\sigma_{\mathrm{d}}(H_\omega) = \varnothing$ for P-a.e. $\omega \in \Omega$.

PROOF. Assume $\lambda \in \Sigma_{\mathrm{d}}$. Then there exists an $\varepsilon > 0$ such that $[\lambda - \varepsilon, \lambda + \varepsilon] \cap \Sigma = \varnothing$ and

$$P_\omega(\{\lambda\}) = E_\omega(\lambda + \varepsilon) - E_\omega(\lambda - \varepsilon) \tag{5.1.42}$$

is the projection onto the eigenspace of H_ω associated with λ. Since $\{P_\omega(\{\lambda\})\}_{\omega\in\Omega}$ is ergodic, Lemma 5.1.9 applies. Moreover, since λ is an eigenvalue of H_ω, $\dim\{\mathrm{Ran}[P_\omega(\{\lambda\})]\} \neq 0$ P-a.s. Thus $\dim\{\mathrm{Ran}[P_\omega(\{\lambda\})]\} = \infty$ P-a.s. which contradicts the assumption that $\lambda \in \Sigma_{\mathrm{d}}$. Thus $\Sigma_{\mathrm{d}} = \varnothing$. ■

Theorem 5.1.11. *Let $\{H_\omega\}_{\omega\in\Omega}$ be an ergodic family of P-a.s. self-adjoint operators in $\mathscr{H}$. Fix $\lambda \in \mathbb{R}$. Then λ is an eigenvalue of H_ω either with probability zero or probability one and the dimension of the corresponding eigenspace is P-a.s. constant. If, in addition, the associated family of unitary operators $\{U_j\}_{j\in I}$ is complete, then the dimension of the eigenspace corresponding to λ is P-a.s. zero or infinite.*

Proof. Let

$$P_\omega(\{\lambda\}) = s\text{-}\lim_{\varepsilon\downarrow 0}\,[E_\omega(\lambda+\varepsilon) - E_\omega(\lambda-\varepsilon)]. \tag{5.1.43}$$

Then

$$\dim\{\mathrm{Ran}[P_\omega(\{\lambda\})]\} = \mathrm{Tr}[P_\omega(\{\lambda\})]. \tag{5.1.44}$$

Since $\{E_\omega(\mu)\}_{\omega\in\Omega}$ is ergodic for all $\mu \in \mathbb{R}$, $\{P_\omega(\{\lambda\})\}_{\omega\in\Omega}$ is also ergodic. Thus

$$\begin{aligned}\dim\{\mathrm{Ran}[P_{T_j\omega}(\{\lambda\})]\} &= \mathrm{Tr}[P_{T_j\omega}(\{\lambda\})] = \mathrm{Tr}[U_jP_\omega(\{\lambda\})U_j^{-1}]\\ &= \mathrm{Tr}[P_\omega(\{\lambda\})] = \dim\{\mathrm{Ran}[P_\omega(\{\lambda\})]\}\end{aligned} \tag{5.1.45}$$

is a measurable function invariant under $\{T_j\}_{j\in I}$. Consequently, $\dim\{\mathrm{Ran}[P_\omega(\{\lambda\})]\}$ is P-a.s. constant. If, in addition, $\{U_j\}_{j\in I}$ is complete, then Lemma 5.1.9 proves the last assertion in the theorem. ■

Theorem 5.1.10 shows that P-a.s. there are no isolated eigenvalues of H_ω of finite multiplicity. Theorem 5.1.11, on the other hand, shows that each $\lambda \in \mathbb{R}$ is P-a.s. no eigenvalue of H_ω with finite multiplicity. Clearly, this does not imply that there are no eigenvalues of finite multiplicity P-a.s. In fact, Theorem 5.1.11 asserts, for any $\lambda \in \mathbb{R}$, the existence of a subset $\Omega_\lambda \subseteq \Omega$ with $P(\Omega_\lambda) = 1$ such that λ is no eigenvalue of finite multiplicity of H_ω, $\omega \in \Omega_\lambda$. Thus for all $\omega \in \bigcap_{\lambda\in\mathbb{R}}\Omega_\lambda$, provided $\bigcap_{\lambda\in\mathbb{R}}\Omega_\lambda \neq \varnothing$, H_ω has no eigenvalues of finite multiplicity. But in general $P(\bigcap_{\lambda\in\mathbb{R}}\Omega_\lambda) < 1$. (In fact, in certain one-dimensional systems it is known that $P(\bigcap_{\lambda\in\mathbb{R}}\Omega_\lambda) = 0$ [217].)

We also emphasize that in general $\sigma_{\mathrm{p}}(H_\omega)$ strongly varies in $\omega \in \Omega$. Only its closure $\overline{\sigma_{\mathrm{p}}(H_\omega)}$ equals a nonrandom set Σ_{p} P-a.s.

III.5.2 Random Point Interactions in Three Dimensions

The main purpose of this section is to construct random point interactions in three dimensions, to show that the results of Sect. 5.1 apply and to investigate the spectrum of this model.

Let $(\Omega, \mathscr{F}, P)$ be a complete probability space. Assume $\{Y(\omega)\}_{\omega\in\Omega}$ to be a countable random subset of $\mathbb{R}^3$ of the form $Y(\omega) = \{y_j(\omega) \in \mathbb{R}^3 \mid j \in \mathbb{N}\}$ where the $y_j, j \in \mathbb{N}$, are $\mathbb{R}^3$-valued random variables such that

$$\inf_{\substack{j, j' \in \mathbb{N} \\ j \neq j'}} |y_j(\omega) - y_{j'}(\omega)| = d > 0, \qquad \omega \in \Omega. \tag{5.2.1}$$

Moreover, let $\alpha(\omega) = \{\alpha_{y_j}(\omega) \in \mathbb{R} \,|\, j \in \mathbb{N}\}$ be an Y-indexed family of real-valued random variables. Then

$$H_\omega = -\Delta_{\alpha(\omega), Y(\omega)}, \qquad \omega \in \Omega, \tag{5.2.2}$$

is a well-defined self-adjoint operator in $L^2(\mathbb{R}^3)$ whose resolvent is given by (1.1.6) with (α, Y) replaced by $(\alpha(\omega), Y(\omega))$. In fact, at this point, H_ω is just the usual Hamiltonian of Sect. 1.1 depending on an additional parameter ω. Since we are particularly interested in the case where $\{H_\omega\}_{\omega \in \Omega}$ is an ergodic family, we have to strengthen our hypotheses considerably. In fact, we shall consider a particularly simple case where $Y(\omega)$ is the level one stochastic set $\Lambda(\omega)$ of a countable family of independent, identically distributed (i.i.d.) $\{0, 1\}$-valued random variables $\{X_\lambda\}_{\lambda \in \Lambda}$, Λ the Bravais lattice (1.4.3). In other words,

$$\Lambda(\omega) = \{\lambda \in \Lambda \,|\, X_\lambda(\omega) = 1\}, \qquad \omega \in \Omega, \tag{5.2.3}$$

represents the occupied sites in Λ. We also assume $\{\alpha_\lambda\}_{\lambda \in \Lambda}$ to be i.i.d. random variables with $\operatorname{supp}(P_{\alpha_0})$ compact (P_{α_0} the distribution of α_0, i.e., $P_{\alpha_0}(A) = P(\alpha_0^{-1}(A))$, $A \in \mathscr{F}$). From now on the *random point interaction* Hamiltonian H_ω is always given by

$$H_\omega = -\Delta_{\alpha(\omega), \Lambda(\omega)}, \qquad \omega \in \Omega, \tag{5.2.4}$$

with $\alpha(\omega)$ as just defined above and $\Lambda(\omega)$ described in (5.2.3). This means that in the notation of Theorem 1.4.4 we have restricted ourselves to the simplest case where $Y = \{0\}$. In the special case where $\Lambda(\omega) = \Lambda$, $\omega \in \Omega$, H_ω models point interaction alloys with randomly distributed coupling constants over the lattice Λ in the one-body approximation . In the general case, H_ω describes in addition random point defects.

Since $\{\alpha_\lambda\}_{\lambda \in \Lambda}$, $\{X_\lambda\}_{\lambda \in \Lambda}$ are i.i.d. random variables we can think of $(\Omega, \mathscr{F}, P)$ as the canonical space for the joint field $\{\alpha_\lambda, X_\lambda\}_{\lambda \in \Lambda}$, i.e., $(\Omega, \mathscr{F}, P) = \prod_{\lambda \in \Lambda} (\Omega_\lambda, \mathscr{F}_\lambda, P_\lambda)$ where $(\Omega_\lambda, \mathscr{F}_\lambda, P_\lambda)$, $\lambda \in \Lambda$, are identical copies of the same probability space. Then the points $\omega \in \Omega$ can be looked upon as points in a discrete Cartesian product $\omega = \Pi_{\lambda \in \Lambda} \omega_\lambda$ and we call ω_λ the λth component of ω. In this representation $\omega_\lambda = (\alpha_\lambda(\omega), X_\lambda(\omega))$.

Next let $\{T_\lambda\}_{\lambda \in \Lambda}$ be the *shift operator* on Ω defined by

$$(T_{\lambda'}\omega)_\lambda = \omega_{\lambda - \lambda'}, \qquad \omega \in \Omega, \quad \lambda, \lambda' \in \Lambda. \tag{5.2.5}$$

We remark that

$$\alpha_\lambda(T_{\lambda'}\omega) = \alpha_{\lambda - \lambda'}(\omega), \qquad X_\lambda(T_{\lambda'}\omega) = X_{\lambda - \lambda'}(\omega), \qquad \omega \in \Omega, \quad \lambda, \lambda' \in \Lambda. \tag{5.2.6}$$

Then T_λ is a measurable transformation which preserves P. Moreover, let $A \in \mathscr{F}$ be a $\{T_\lambda\}_{\lambda \in \Lambda}$ invariant set, i.e., $T_\lambda^{-1}(A) = A$, $\lambda \in \Lambda$. Then A is in the tail σ-algebra (cf. Appendix I) of the random variables $\{\alpha_\lambda, X_\lambda\}_{\lambda \in \Lambda}$. Since α_λ, X_λ, $\lambda \in \Lambda$, are independent, we get $P(A) = 0$ or $P(A) = 1$ be Kolmogorov's 0–1 law (cf. Appendix I). Thus $\{T_\lambda\}_{\lambda \in \Lambda}$ is a family of measure preserving, ergodic transformations. Let $\{U_\lambda\}_{\lambda \in \Lambda}$ denote the family of unitary translation operators in $L^2(\mathbb{R}^3)$

$$(U_\lambda g)(x) = g(x - \lambda), \qquad g \in L^2(R^3), \quad \lambda \in \Lambda. \tag{5.2.7}$$

Clearly, $\{U_\lambda\}_{\lambda \in \Lambda}$ is complete in the sense of Sect. 5.1. We get

Lemma 5.2.1. *Let $\{H_\omega\}_{\omega \in \Omega}$ be defined as in* (5.2.4). *Then $\{H_\omega\}_{\omega \in \Omega}$ is an ergodic family of self-adjoint operators in $L^2(\mathbb{R}^3)$ and*

$$U_\lambda H_\omega U_\lambda^{-1} = H_{T_\lambda \omega}, \qquad \omega \in \Omega, \quad \lambda \in \Lambda. \tag{5.2.8}$$

PROOF. Measurability of $\{H_\omega\}_{\omega \in \Omega}$ simply follows from Theorem 1.1.1 and Lemma 5.1.3. Moreover, approximating H_ω by scaled, short-range interactions $H_{\varepsilon, \Lambda(\omega)}$ with

$$\lambda_\lambda(\varepsilon, T_{\lambda'}\omega) = \lambda_{\lambda - \lambda'}(\varepsilon, \omega), \qquad \omega \in \Omega, \quad \lambda, \lambda' \in \Lambda, \tag{5.2.9}$$

in norm resolvent sense (cf. Theorem 1.2.1), observing (5.2.6), we infer

$$U_\lambda(H_{\varepsilon, \Lambda(\omega)} - k^2)^{-1} U_\lambda^{-1} = (H_{\varepsilon, \Lambda(T_\lambda \omega)} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \quad \omega \in \Omega, \quad \lambda \in \Lambda, \tag{5.2.10}$$

and hence

$$U_\lambda(H_\omega - k^2)^{-1} U_\lambda^{-1} = (H_{T_\lambda \omega} - k^2)^{-1}, \qquad k^2 \in \mathbb{C} - \mathbb{R}, \quad \omega \in \Omega, \quad \lambda \in \Lambda. \tag{5.2.11}$$

■

Thus Theorems 5.1.5, 5.1.8, 5.1.10, and 5.1.11 immediately apply and we get

Theorem 5.2.2. *Let $\{H_\omega\}_{\omega \in \Omega}$ be defined as in* (5.2.4). *Then $\sigma(H_\omega)$, $\sigma_{\mathrm{ess}}(H_\omega)$, $\sigma_{\mathrm{c}}(H_\omega)$, $\sigma_{\mathrm{ac}}(H_\omega)$, $\sigma_{\mathrm{sc}}(H_\omega)$,* and *$\sigma_{\mathrm{p}}(H_\omega)$ all equal certain nonrandom sets Σ, Σ_{ess}, Σ_{c}, Σ_{ac}, Σ_{sc}, and $\Sigma_{\mathrm{p}} \subseteq \mathbb{R}$ for P-a.e. $\omega \in \Omega$. Moreover, $\sigma_{\mathrm{d}}(H_\omega) = \varnothing$ for P-a.e. $\omega \in \Omega$. In addition, for any $\tau \in \mathbb{R}$ there exists a subset $\Omega_\tau \subseteq \Omega$ with $P(\Omega_\tau) = 1$ such that τ is no eigenvalue of finite multiplicity of H_ω, $\omega \in \Omega_\tau$.*

In the rest of this section we shall investigate $\Sigma = \sigma(H_\omega)$ for P-a.e. $\omega \in \Omega$ in more detail. For this purpose we introduce some more notations. Let us denote $\Phi(\omega) = \{\alpha_\lambda(\omega), X_\lambda(\omega)\}_{\lambda \in \Lambda}$, $\omega \in \Omega$. Then $\Phi(\omega)$ determines the positions and strengths of the random potential sources, hence we call $\Phi(\omega)$ the *stochastic potential.* By $H(\Phi(\omega))$ we denote the operator $-\Delta_{\alpha(\omega), \Lambda(\omega)}$ with positions and strengths given by $\Phi(\omega)$, i.e., $\alpha(\omega) = \{\alpha_\lambda(\omega)\}_{\lambda \in \Lambda}$, $\Lambda(\omega) = \{\lambda \in \Lambda \mid X_\lambda(\omega) = 1\}$. A sequence $\phi = \{(\xi_\lambda, \eta_\lambda) \in \mathrm{supp}(P_{\alpha_0}) \times \{0, 1\}\}_{\lambda \in \Lambda}$ is called an *admissible potential.* The set of all admissible potentials is denoted by $\mathscr{A}$. For each $\phi \in \mathscr{A}$ we denote by $H(\phi)$ the operator $-\Delta_{\alpha, \Lambda(\phi)}$ with $\alpha = \{\xi_\lambda\}_{\lambda \in \Lambda}$, $\Lambda(\phi) = \{\lambda \in \Lambda \mid \eta_\lambda = 1\}$. Next we call $\phi \in \mathscr{A}$ *periodic* (with periods L_1, L_2, L_3) if there exist linearly independent $L_m \in \Lambda - \{0\}$, $m = 1, 2, 3$, such that

$$\xi_{\lambda + L_m} = \xi_\lambda, \qquad \eta_{\lambda + L_m} = \eta_\lambda, \qquad \lambda \in \Lambda, \quad m = 1, 2, 3. \tag{5.2.12}$$

Finally, let $\mathscr{P}$ denote the set of all periodic, admissible potentials.

Given these preliminaries we are able to formulate

Theorem 5.2.3. *Let $\Phi(\omega)$ be the stochastic potential defined above. Then*

(i)
$$\sigma(H(\phi)) \subseteq \Sigma, \qquad \phi \in \mathscr{A}. \tag{5.2.13}$$

(ii)
$$\Sigma = \bigcup_{\phi \in \mathscr{A}} \sigma(H(\phi)) = \overline{\bigcup_{\phi \in \mathscr{P}} \sigma(H(\phi))}, \tag{5.2.14}$$

where $\Sigma = \sigma(H(\Phi(\omega)))$ for P-a.e. $\omega \in \Omega$.

Proof. Let $\Phi(\omega)$ be the given stochastic potential and let $\phi = \{(\xi_\lambda, \eta_\lambda)\}_{\lambda \in \Lambda} \in \mathscr{A}$. Then (1.1.6) and (1.1.7) imply

$$(H(\phi) - k^2)^{-1} = G_k + \sum_{\lambda, \lambda' \in \Lambda} \{[T_k(\phi)]^{-1} - 1_{[\Lambda(\phi)]^c}\}_{\lambda,\lambda'} (\overline{G_k(\cdot - y_{\lambda'})}, \cdot) G_k(\cdot - y_\lambda),$$
$$k^2 \in \rho(H(\phi)), \quad \operatorname{Im} k > 0. \tag{5.2.15}$$

Here 1_M denotes the identity on a set $M \subseteq \Lambda$, $[\Lambda(\phi)]^c = \Lambda - \Lambda(\phi)$, and

$$T_k(\phi) = \Gamma_{\xi, \Lambda(\phi)}(k) + 1_{[\Lambda(\phi)]^c},$$
$$[\Gamma_{\xi,\Lambda(\phi)}(k)]_{\lambda\lambda'} = \left(\xi_\lambda - \frac{ik}{4\pi}\right)\delta_{\lambda\lambda'} - \tilde{G}_k(\lambda - \lambda'), \qquad \lambda, \lambda' \in \Lambda(\phi), \quad \operatorname{Im} k > 0. \tag{5.2.16}$$

Next let

$$\Omega^1 = \{\omega \in \Omega \,|\, \sigma(H(\Phi(\omega))) \equiv \Sigma\}. \tag{5.2.17}$$

By Theorem 5.2.2, Ω^1 has probability one, i.e., $P(\Omega^1) = 1$. Define

$$\Omega_n^\phi = \{\omega \in \Omega \,|\, |\alpha_\lambda(\omega) - \xi_\lambda| < n^{-1}, |\lambda| \leq n\}, \qquad n \in \mathbb{N}. \tag{5.2.18}$$

Since α_λ are i.i.d. random variables we get

$$\begin{aligned} P(\Omega_n^\phi) &= \prod_{|\lambda| \leq n} P(\{\omega \in \Omega \,|\, |\alpha_\lambda(\omega) - \xi_\lambda| < n^{-1}\}) \\ &= \prod_{|\lambda| \leq n} P(\{\omega \in \Omega \,|\, |\alpha_0(\omega) - \xi_\lambda| < n^{-1}\}), \qquad n \in \mathbb{N}. \end{aligned} \tag{5.2.19}$$

By assumption $\xi_\lambda \in \operatorname{supp}(P_{\alpha_0})$, $\lambda \in \Lambda$. If we assume that

$$P(\{\omega \in \Omega \,|\, |\alpha_0(\omega) - \xi_\lambda| < n^{-1}\}) = 0 \text{ for some } n \in \mathbb{N} \text{ then}$$
$$P_{\alpha_0}((\xi_\lambda - n^{-1}, \xi_\lambda + n^{-1})) = 0$$

would imply the contradiction $\xi_\lambda \notin \operatorname{supp}(P_{\alpha_0})$. Hence $P(\{\omega \in \Omega \,|\, |\alpha_0(\omega) - \xi_\lambda| < n^{-1}\}) > 0$ implying $P(\Omega_n^\phi) > 0$. In particular, $\Omega^1 \cap \Omega_n^\phi \neq \varnothing$ (since otherwise $P(\Omega^1 \cup \Omega_n^\phi) = 1 + P(\Omega_n^\phi) > 1$ yields a contradiction). Pick $\omega_n \in \Omega^1 \cap \Omega_n^\phi$. Then

$$\sigma(H(\Phi(\omega_n))) = \Sigma. \tag{5.2.20}$$

Using the definition of Ω_n^ϕ, one then proves that

$$\{[T_{i\kappa}(\Phi(\omega_n))]^{-1} - 1_{[\Lambda(\Phi(\omega_n))]^c}\} \xrightarrow[n \to \infty]{s} [T_{i\kappa}(\phi)]^{-1} - 1_{[\Lambda(\phi)]^c},$$
$$\kappa > 0 \quad \text{large enough}, \tag{5.2.21}$$

in $l^2(\Lambda)$. Here $T_k(\Phi(\omega_n))$ (which is defined in analogy to (5.2.16)) is associated with $H(\Phi(\omega_n))$ like $T_k(\phi)$ is associated with $H(\phi)$ (cf. (5.2.15)). Similarly, $\Lambda(\Phi(\omega_n)) =$

$\{\lambda \in \Lambda | X_\lambda(\omega_n) = 1\}$. Assertion (5.2.21) is shown by first proving $T_{i\kappa}(\Phi(\omega_n)) \xrightarrow[n\to\infty]{s} T_{i\kappa}(\phi)$ on vectors of $l^2(\Lambda)$ of compact support (i.e., on $l_0^2(\Lambda)$). Since $T_{i\kappa}(\Phi(\omega_n))$, $T_{i\kappa}(\phi)$, $\kappa > 0$, are bounded and self-adjoint, this finally proves (5.2.21). Using (5.2.21) and the fact that $\{(\overline{G_k(\cdot - \lambda), f})\}_{\lambda \in \Lambda} \in l^2(\Lambda)$, $f \in L^2(\mathbb{R}^3)$ (cf. (1.1.24) and the following arguments) one proves that $H(\Phi(\omega_n))$ converges in weak (and hence in strong) resolvent sense to $H(\phi)$ as $n \to \infty$. This finally implies, using Theorem VIII.24 of [388], that

$$\sigma(H(\phi)) \subseteq \overline{\bigcup_{n\in\mathbb{N}} \sigma(H(\Phi(\omega_n)))} = \Sigma. \tag{5.2.22}$$

In particular, (5.2.22) implies

$$\bigcup_{\phi \in \mathscr{A}} \sigma(H(\phi)) \subseteq \Sigma. \tag{5.2.23}$$

Next let $\omega^1 \in \Omega^1$ and let

$$\phi^1 = \{(\xi_\lambda, \eta_\lambda) \in \operatorname{supp}(P_{\alpha_0}) \times \{0, 1\}\}_{\lambda \in \Lambda} = \Phi(\omega^1) \tag{5.2.24}$$

with

$$\eta_\lambda = X_\lambda(\omega^1), \qquad \xi_\lambda = \alpha_\lambda(\omega^1), \qquad \lambda \in \Lambda. \tag{5.2.25}$$

Then $\phi^1 \in \mathscr{A}$ and thus

$$\bigcup_{\phi \in \mathscr{A}} \sigma(H(\phi)) \supseteq \sigma(H(\phi^1)) = \sigma(H(\Phi(\omega^1))) = \Sigma. \tag{5.2.26}$$

Together with (5.2.23) this proves the first assertion in (ii). To prove the second assertion in (ii) we first prove that for any $\phi \in \mathscr{A}$ we can find a sequence $\{\phi_n\}_{n\in\mathbb{N}} \subset \mathscr{P}$ such that $H(\phi_n)$ converges to $H(\phi)$ in strong resolvent sense as $n \to \infty$. For that purpose we define

$$\begin{aligned} &(\phi_n)_\lambda = (\xi_\lambda^n, \eta_\lambda^n) = (\xi_\lambda, \eta_\lambda), \qquad \lambda \in \Lambda_n, \\ &\quad \Lambda_n = \{n_1 a_1 + n_2 a_2 + n_3 a_3 \in \Lambda \,|\, |n_m| \le n, n_m \in \mathbb{Z}, m = 1, 2, 3\}, \qquad n \in \mathbb{N}, \end{aligned} \tag{5.2.27}$$

and continue periodically outside Λ_n. Take $\psi \in l_0^2(\Lambda) = \{g \in l^2(\Lambda) | \operatorname{supp}(g)$ compact$\}$.Then

$$\|[\Gamma_{\xi,\Lambda(\phi_n)}(k) - \Gamma_{\xi,\Lambda(\phi)}(k)]\psi\|^2 = \sum_{\lambda\in\Lambda} |\xi_\lambda^n - \xi_\lambda|^2 |\psi(\lambda)|^2 \xrightarrow[n\to\infty]{} 0, \tag{5.2.28}$$

since $\xi_\lambda^n = \xi_\lambda$ for $\lambda \in \Lambda_n$ and ψ has compact support. Hence $T_k(\phi_n) \xrightarrow[n\to\infty]{s} T_k(\phi)$. Take $k = i\kappa$, $\kappa > 0$. Then $T_{i\kappa}(\phi_n)$ and $T_{i\kappa}(\phi)$ are bounded and self-adjoint, implying convergence of $T_{i\kappa}(\phi_n)$ to $T_{i\kappa}(\phi)$ in the strong resolvent sense as $n \to \infty$. As in the argument following (5.2.21) this proves that $H(\phi_n)$ converges to $H(\phi)$ in strong resolvent sense as $n \to \infty$. The result together with Theorem VIII.24 of [388] shows

$$\sigma(H(\phi)) \subseteq \overline{\bigcup_{n\in\mathbb{N}} \sigma(H(\phi_n))}. \tag{5.2.29}$$

Using (5.2.26) this implies

$$\Sigma \subseteq \overline{\bigcup_{n\in\mathscr{P}} \sigma(H(\phi_n))}. \tag{5.2.30}$$

On the other hand, $\mathscr{P} \subseteq \mathscr{A}$ and (5.2.23) then shows

$$\Sigma \supseteq \bigcup_{\phi \in \mathscr{P}} \sigma(H(\phi)). \tag{5.2.31}$$

Taking closures, this and (5.2.30) complete the proof. ■

Theorem 5.2.3(ii) shows, in particular, that Σ only depends on $\operatorname{supp}(P_{\alpha_0})$ and not on other properties of P_{α_0}. In addition, it shows that Σ has a band structure of the type $\Sigma = \overline{\bigcup_{m \in \mathbb{N}} [a_m, b_m]}$, $a_m < b_m$, $m \in \mathbb{N}$, and hence Σ is the closure of the open set $\bigcup_{m \in \mathbb{N}} (a_m, b_m)$.

Next we turn to a detailed study of the negative part of the spectrum of $H(\Phi(\omega))$ as one removes point interactions.

Lemma 5.2.4. *Let* $\mu = \inf[\operatorname{supp}(P_{\alpha_0})]$, $\nu = \sup[\operatorname{supp}(P_{\alpha_0})]$, *and let* Λ_n, $n \in \mathbb{N}$, *be defined as in* (5.2.27). *Let* $\phi_n \in \mathscr{A}$ *be the admissible potential*

$$\phi_n = \{(\xi_\lambda, \eta_\lambda) \in \operatorname{supp}(P_{\alpha_0}) \times \{0, 1\}\}_{\lambda \in \Lambda},$$
$$\eta_\lambda = 1, \quad \lambda \in \Lambda_n, \quad \eta_\lambda = 0, \quad \lambda \in \Lambda - \Lambda_n, \quad n \in \mathbb{N}. \tag{5.2.32}$$

Then

$$\sigma(H(\phi_n)) \cap (-\infty, 0) \subseteq [E_0^{\mu, \Lambda}(0), E_0^{\nu, \Lambda}(\theta_0)] \cap (-\infty, 0), \qquad n \in \mathbb{N}, \tag{5.2.33}$$

where we used the terminology of Theorem 1.4.5 *on the right-hand side of* (5.2.33).

Proof. By Sect. II.1.1, the negative eigenvalues $E_{l,n} = k_{l,n}^2 < 0$, $l = 1, \ldots, N_n$, of $H(\phi_n)$ are in one-to-one correspondence with zero eigenvalues of $\Gamma_{\xi, \Lambda(\phi_n)}(k_{l,n})$, $l = 1, \ldots, N_n$. Denote by $E_{\max,n}(\xi)$ (resp. $E_{\min,n}(\xi)$) the largest (resp. smallest) of these eigenvalues $E_{l,n}$, $l = 1, \ldots, N_n$. Because all eigenvalues of $\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa)$ are strictly increasing in κ, $\kappa > 0$, we get that $E_{\max,n}(\xi)$ (resp. $E_{\min,n}(\xi)$) is the unique eigenvalue such that

$$\sup[\sigma(\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa))] = 0 \quad (\text{resp. } \inf[\sigma(\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa))] = 0), \qquad \kappa > 0, \tag{5.2.34}$$

for $k^2 = -\kappa^2$. Moreover, by the monotonicity of $\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa)$, $\kappa > 0$, with respect to ξ and by Rayleigh's theorem ([391], p. 364) we infer

$$\sup[\sigma(\Gamma_{\nu, \Lambda}(i\kappa))] \geq \sup[\sigma(\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa))],$$
$$\inf[\sigma(\Gamma_{\mu, \Lambda}(i\kappa))] \leq \inf[\sigma(\Gamma_{\xi, \Lambda(\phi_n)}(i\kappa))], \qquad \kappa > 0. \tag{5.2.35}$$

Clearly, $E_0^{\nu, \Lambda}(\theta_0)$ (resp. $E_0^{\mu, \Lambda}(0)$) is the value of $k^2 = -\kappa^2$ for which $\sup[\sigma(\Gamma_{\nu, \Lambda}(i\kappa))] = 0$ (resp. $\inf[\sigma(\Gamma_{\mu, \Lambda}(i\kappa))] = 0$) (cf. Theorem 1.4.5). Thus

$$E_0^{\mu, \Lambda}(0) \leq E_{\min,n}(\xi) \leq E_{\max,n}(\xi) \leq E_0^{\nu, \Lambda}(\theta_0), \qquad \xi \in \operatorname{supp}(P_{\alpha_0}), \qquad n \in \mathbb{N}, \tag{5.2.36}$$

and hence Theorem 1.4.5 implies (5.2.33). ■

Next we state

Lemma 5.2.5. *Assume the hypotheses of Lemma* 5.2.4. *Let* $\tilde{\Lambda} \subset \Lambda$ *and define* $\phi_n^{\tilde{\Lambda}} \in \mathscr{A}$ *to be the admissible potential*

$$\phi_n^{\tilde{\Lambda}} = \{(\xi_\lambda, \eta_\lambda) \in \operatorname{supp}(P_{\alpha_0}) \times \{0, 1\}\}_{\lambda \in \Lambda},$$
$$\eta_\lambda = 1, \quad \lambda \in \Lambda_n - \tilde{\Lambda}, \quad \eta_\lambda = 0, \quad \lambda \notin \Lambda_n - \tilde{\Lambda}, \quad n \in \mathbb{N}. \tag{5.2.37}$$

Then

$$\sigma(H(\phi_n^{\tilde{\Lambda}})) \subseteq \sigma(H(\phi_n)), \qquad n \in \mathbb{N}. \tag{5.2.38}$$

PROOF. Since $\Gamma_{\xi,\Lambda(\phi_n^{\tilde{\Lambda}})}(k)$ is the restriction of $\Gamma_{\xi,\Lambda(\phi_n)}(k)$ to a subspace, it follows from Rayleigh's theorem ([391], p. 364) that

$$\begin{aligned} &\sup[\sigma(\Gamma_{\xi,\Lambda(\phi_n^{\tilde{\Lambda}})}(i\kappa))] \leq \sup[\sigma(\Gamma_{\xi,\Lambda(\phi_n)}(i\kappa))], \\ &\inf[\sigma(\Gamma_{\xi,\Lambda(\phi_n^{\tilde{\Lambda}})}(i\kappa))] \geq \inf[\sigma(\Gamma_{\xi,\Lambda(\phi_n)}(i\kappa))], \qquad \kappa > 0. \end{aligned} \tag{5.2.39}$$

Define $E_{\min,n}^{\tilde{\Lambda}}(\xi)$, $E_{\max,n}^{\tilde{\Lambda}}(\xi)$ in analogy to $E_{\min,n}(\xi)$, $E_{\max,n}(\xi)$ in the proof of Lemma 5.2.4 (replacing ϕ_n by $\phi_n^{\tilde{\Lambda}}$). The fact that all eigenvalues of $\Gamma_{\xi,\Lambda(\phi_n)}(i\kappa)$, $\Gamma_{\xi,\Lambda(\phi_n^{\tilde{\Lambda}})}(i\kappa)$ are strictly increasing in κ, $\kappa > 0$, together with (5.2.39) then yields

$$E_{\min,n}(\xi) \leq E_{\min,n}^{\tilde{\Lambda}}(\xi) \leq E_{\max,n}^{\tilde{\Lambda}}(\xi) \leq E_{\max,n}(\xi), \qquad \xi \in \operatorname{supp}(P_{\alpha_0}), \quad n \in \mathbb{N}. \tag{5.2.40}$$

This proves

$$\{\sigma(H(\phi_n^{\tilde{\Lambda}})) \cap (-\infty, 0)\} \subset \{\sigma(H(\phi_n)) \cap (-\infty, 0)\}, \qquad n \in \mathbb{N}. \tag{5.2.41}$$

But since both $H(\phi_n^{\tilde{\Lambda}})$ and $H(\phi_n)$ only describe a finite number of point interactions

$$[0, \infty) \subseteq \{\sigma(H(\phi_n^{\tilde{\Lambda}})) \cap \sigma(H(\phi_n))\}, \qquad n \in \mathbb{N}, \tag{5.2.42}$$

and the proof is complete. ■

Lemma 5.2.6. *Let* $\mu = \inf[\operatorname{supp}(P_{\alpha_0})]$, $\nu = \sup[\operatorname{supp}(P_{\alpha_0})]$. *Then*

$$\Sigma \cap (-\infty, 0) \subseteq [E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)] \cap (-\infty, 0). \tag{5.2.43}$$

In particular, if $\nu < \alpha_{0,\Lambda}$ (*cf.* (1.4.101)) then

$$\Sigma \cap [E_0^{\nu,\Lambda}(\theta_0), 0) = \varnothing. \tag{5.2.44}$$

PROOF. Let ξ in ϕ_n, $\phi_n^{\tilde{\Lambda}}$ of Lemmas 5.2.4 and 5.2.5 be periodic with periods $L_1, L_2, L_3 \in \Lambda - \{0\}$. Arguing as in the proof of Theorem 5.2.3 we infer that $H(\phi_n) \to H(\phi)$ and $H(\phi_n^{\tilde{\Lambda}}) \to H(\phi^{\tilde{\Lambda}})$ in strong resolvent sense as $n \to \infty$. Here

$$\begin{aligned} \phi &= \{(\xi_\lambda, \eta_\lambda) \in \operatorname{supp}(P_{\alpha_0}) \times \{0, 1\} | \eta_\lambda = 1, \lambda \in \Lambda\}, \\ \phi^{\tilde{\Lambda}} &= \{(\xi_\lambda, \eta_\lambda) \in \operatorname{supp}(P_{\alpha_0}) \times \{0, 1\} | \eta_\lambda = 1, \lambda \in \Lambda - \tilde{\Lambda}, \eta_\lambda = 0, \lambda \notin \Lambda - \tilde{\Lambda}\}, \\ \xi_{\lambda+L_m} &= \xi_\lambda, \qquad \lambda \in \Lambda, \quad m = 1, 2, 3, \end{aligned} \tag{5.2.45}$$

(i.e., $\Lambda(\phi) = \Lambda$, $\Lambda(\phi^{\tilde{\Lambda}}) = \Lambda - \tilde{\Lambda}$). By Lemmas 5.2.4 and 5.2.5 we get

$$\begin{aligned} \sigma(H(\phi^{\tilde{\Lambda}})) \cap (-\infty, 0) &\subseteq \sigma(H(\phi)) \cap (-\infty, 0) \\ &\subseteq [E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)] \cap (-\infty, 0). \end{aligned} \tag{5.2.46}$$

Next let $\Phi(\omega) = \{\alpha_\lambda(\omega), X_\lambda(\omega)\}_{\lambda \in \Lambda}$ be a stochastic potential and $\Lambda(\omega) = \{\lambda \in \Lambda | X_\lambda(\omega) = 1\}$. By Theorem 5.2.2 we have $\sigma(H(\Phi(\omega^1))) = \Sigma$ for some $\omega^1 \in \Omega$. Let us now choose

$$\tilde{\Lambda} = [\Lambda(\omega^1)]^c, \qquad \xi_\lambda = (\alpha(\omega^1))_\lambda, \qquad \lambda \in \Lambda. \tag{5.2.47}$$

Then $\Phi(\omega^1) = \phi^{\tilde{\Lambda}}$ and hence (5.2.46) implies (5.2.43). ■

Next we state

Lemma 5.2.7. *Let* $-\Delta_{\alpha, Y+\Lambda}$ *be the operator defined in Theorem* 1.4.3 *and assume* $\alpha_- \leq \alpha_j \leq \alpha_+$, $\alpha_\pm \in \mathbb{R}, j = 1, \ldots, N$. *Let* $\tilde{E} \in \sigma(-\Delta_{\alpha, Y+\Lambda})$. *Then there exists an* $\tilde{\alpha} \in [\alpha_-, \alpha_+]$ *such that* $\tilde{E} \in \sigma(-\Delta_{\tilde{\alpha}, \Lambda})$ *(where* $-\Delta_{\tilde{\alpha}, \Lambda}$ *is defined in Theorem* 1.4.4).

PROOF. Let $V_j = V \in C_0^\infty(\mathbb{R}^3)$ be real-valued, $j = 1, \ldots, N$, and $V \leq 0$. Denote by $H_{\varepsilon, Y+\Lambda}$ (resp. by $H_{\varepsilon, \Lambda}$) the operators in (1.4.116) which by Theorem 1.2.1 approximate $-\Delta_{\alpha, Y+\Lambda}$ (resp. $-\Delta_{\gamma, \Lambda}$), $\gamma \in \mathbb{R}$, in norm resolvent sense as $\varepsilon \downarrow 0$. In addition, we assume $H = -\Delta \dot{+} V$ to be in case II with ϕ the corresponding zero-energy resonance function and choose

$$\lambda_j(\varepsilon) = 1 - |(v, \phi)|^2 \alpha_j \varepsilon, \qquad \varepsilon > 0, \quad j = 1, \ldots, N, \tag{5.2.48}$$

in $H_{\varepsilon, Y+\Lambda}$ and

$$\lambda(\varepsilon) = 1 - |(v, \phi)|^2 \gamma \varepsilon, \qquad \varepsilon > 0, \quad \gamma \in \mathbb{R}, \tag{5.2.49}$$

in $H_{\varepsilon, \Lambda}$. Because of the above-mentioned norm resolvent convergence of $H_{\varepsilon, Y+\Lambda}$ to $-\Delta_{\alpha, Y+\Lambda}$ as $\varepsilon \downarrow 0$, we can choose $\varepsilon > 0$ small enough such that for given $\delta > 0$, the distance $d(\tilde{E}, \sigma(H_{\varepsilon, Y+\Lambda})) \leq \delta$. Next we vary α_j in such a way that either all $\alpha_j \downarrow \alpha_-$ or all $\alpha_j \uparrow \alpha_+, j = 1, \ldots, N$. Using the min–max principle and the fact that the spectrum of $H_{\varepsilon, Y+\Lambda}$ depends continuously on $\alpha_1, \ldots, \alpha_N$, we infer that in the first case $\sigma(H_{\varepsilon, Y+\Lambda})$ moves to the left whereas in the second case it moves to the right. Taking into account that $\sigma(H_{\varepsilon, \Lambda})$ also depends continuously on γ and moves to the left or right if γ is decreased or increased (and that $H_{\varepsilon, \Lambda} = H_{\varepsilon, Y+\Lambda}$ if $\gamma = \alpha_1 = \cdots = \alpha_N$), we get the existence of an $\tilde{\alpha} \in [\alpha_-, \alpha_+]$ such that $d(\tilde{E}, \sigma(\tilde{H}_{\varepsilon, \Lambda})) \leq \delta$ where $\tilde{H}_{\varepsilon, \Lambda}$ equals $H_{\varepsilon, \Lambda}$ with $\gamma = \tilde{\alpha}$. Since $\delta > 0$ was arbitrary we obtain $d(\tilde{E}, \sigma(-\Delta_{\tilde{\alpha}, \Lambda})) = 0$. Since $\sigma(-\Delta_{\tilde{\alpha}, \Lambda})$ is closed we finally get $\tilde{E} \in \sigma(-\Delta_{\tilde{\alpha}, \Lambda})$ as desired. ∎

Now we are ready to give a precise description of Σ. We start with the case where all lattice sites are occupied, i.e., where $P(X_0 = 0) = 0$.

Theorem 5.2.8. *Let* $\mu = \inf[\text{supp}(P_{\alpha_0})]$, $\nu = \sup[\text{supp}(P_{\alpha_0})]$, *and suppose that* $P(X_0 = 0) = 0$. *Moreover, assume that either* $E_0^{\nu, \Lambda}(0) \leq E_0^{\mu, \Lambda}(\theta_0)$ *or that* $\text{supp}(P_{\alpha_0}) = [\mu, \nu]$. *Then*

$$\Sigma = [E_0^{\mu, \nu}(0), E_0^{\nu, \Lambda}(\theta_0)] \cup [E_1^{\mu, \Lambda}, \infty) = \sigma(-\Delta_{\mu, \Lambda}) \cup \sigma(-\Delta_{\nu, \Lambda}). \tag{5.2.50}$$

If, in addition, $\nu < \alpha_{0, \Lambda}$ *then*

$$\Sigma \cap (-\infty, 0) = [E_0^{\mu, \Lambda}(0), E_0^{\nu, \Lambda}(\theta_0)], \qquad E_0^{\nu, \Lambda}(\theta_0) < 0. \tag{5.2.51}$$

If, in addition, $\mu \geq \alpha_{1, \Lambda}$ *then*

$$\Sigma = \sigma(-\Delta_{\mu, \Lambda}). \tag{5.2.52}$$

PROOF. Since (5.2.51) and (5.2.52) are easy consequences of (5.2.50) and the monotonicity of $E_0^{\alpha, \Lambda}(0)$, $E_0^{\alpha, \Lambda}(\theta_0)$ with respect to $\alpha \in \mathbb{R}$, we concentrate on (5.2.50). By (5.2.14) we obviously have

$$\Sigma \supseteq \sigma(-\Delta_{\mu, \Lambda}) \cup \sigma(-\Delta_{\nu, \Lambda}). \tag{5.2.53}$$

On the other hand, by Lemma 5.2.7 we get

$$\sigma(H(\phi)) \subseteq \bigcup_{\alpha \in [\mu, \nu]} \sigma(-\Delta_{\alpha, \Lambda}) = \sigma(-\Delta_{\mu, \Lambda}) \cup \sigma(-\Delta_{\nu, \Lambda}), \qquad \phi \in \mathscr{P}. \tag{5.2.54}$$

By taking the union over all $\phi \in \mathscr{P}$ and the closure the proof is complete. ∎

Finally, we treat the case where $0 < P(X_0 = 0) < 1$ (the case $P(X_0 = 0) = 1$ corresponds to the free Hamiltonian $-\Delta$).

Theorem 5.2.9. *Let* $\mu = \inf[\operatorname{supp}(P_{\alpha_0})]$, $\nu = \sup[\operatorname{supp}(P_{\alpha_0})]$, *and suppose that* $0 < P(X_0 = 0) < 1$. *Moreover, assume that either* $E_0^{\nu,\Lambda}(0) \le E_0^{\mu,\Lambda}(\theta_0)$ *or that* $\operatorname{supp}(P_{\alpha_0}) = [\mu, \nu]$. *Then*

$$\Sigma = [E_0^{\mu,\Lambda}(0), E_0^{\nu,\Lambda}(\theta_0)] \cup [0, \infty) = \sigma(-\Delta_{\mu,\Lambda}) \cup \sigma(-\Delta_{\nu,\Lambda}) \cup [0, \infty). \tag{5.2.55}$$

If, in addition, $\nu < \alpha_{0,\Lambda}$ then (5.2.51) holds If, in addition, $\mu \ge \alpha_{1,\Lambda}$ *then* (5.2.52) *also holds.*

PROOF. For $\Sigma \cap (-\infty, 0)$ we only need to combine Lemma 5.2.6 and (5.2.14). For $\Sigma \cap [0, \infty)$ we argue as follows. Since $P(X_0 = 0) > 0$ by hypothesis, the event that $X_\lambda = 0$ for $\lambda \in \Lambda_n$, $n \in \mathbb{N}$ (cf. 5.2.27)) has positive probability no matter how large n is. Thus

$$\Omega_n = \{\omega \in \Omega \mid \exists \lambda_0 \in \Lambda, \text{ s.t. } \forall \lambda \in \lambda_0 + \Lambda_n\colon X_\lambda = 0\}. \tag{5.2.56}$$

has probability one, $P(\Omega_n) = 1$, since it is invariant with respect to shifts T_λ, $\lambda \in \Lambda$. Thus the set

$$\Omega_\infty = \bigcap_{n \in \mathbb{N}} \Omega_n \tag{5.2.57}$$

has probability one, $P(\Omega_\infty) = 1$. But for $\omega \in \Omega_\infty$ we find subsets $\lambda_0 + \Lambda_m$, $\lambda_0 \in \Lambda$, $m \in \mathbb{N}$ (perhaps far away) of arbitrary large size without point interactions contained in them. Hence a standard argument based on Weyl trial functions (cf., e.g., [391], Ch. XIII) shows that $[0, \infty) \subseteq \sigma(H_\omega)$, $\omega \in \Omega_\infty$. Let Ω^1 be defined as in (5.2.17). Then $\Omega^1 \cap \Omega_\infty \neq \varnothing$ since both sets have probability one. Consequently, for $\omega_0 \in \Omega^1 \cap \Omega_\infty$ we obtain

$$[0, \infty) \subseteq \sigma(H_{\omega_0}) = \Sigma. \tag{5.2.58}$$

■

For $\mu \ge \alpha_{1,\Lambda}$, we get the surprising result that the spectrum of H_ω in Theorems 5.2.8 (where $P(X_0 = 0) = 0$) and 5.2.9 (where $0 < P(X_0 = 0) < 1$) coincides and equals $\sigma(-\Delta_{\mu,\Lambda})$ for P-a.e. $\omega \in \Omega$. In other words, starting from the random Hamiltonian H_ω with centers at the points of the lattice Λ creating point interactions of random strengths and switching off some of the centers in a random way does not change the spectrum in the case where $\mu \ge \alpha_{1,\Lambda}$.

Both Theorems 5.2.8 and 5.2.9 can be viewed as generalizations of the Saxon–Hutner conjecture (cf. Sect. 2.3 and the following one).

III.5.3 Random Point Interactions in One Dimension

Here we derive the analogous results of the foregoing section for random δ- and δ'-interactions in one dimension.

Let $\Lambda = a\mathbb{Z}$, $a > 0$, and consider $-\Delta_{\alpha(\omega),\Lambda}$ and $\Xi_{\beta(\omega),\Lambda}$ in $L^2(\mathbb{R})$ where $\alpha(\omega) = \{\alpha_j(\omega) \in \mathbb{R}\}_{j \in \mathbb{Z}}$, $\beta(\omega) = \{\beta_j(\omega) \in \mathbb{R}\}_{j \in \mathbb{Z}}$, and α_j, β_j, $j \in \mathbb{Z}$ are i.i.d. real-valued random variables on the canonical probability space $(\Omega, \mathscr{F}, P)$. Assume $\text{supp}(P_{\alpha_0})$ and $\text{supp}(P_{\beta_0})$ to be compact. Then Ω is chosen to be $\Omega = [\text{supp}(P_{\alpha_0})]^{\mathbb{Z}}$ (resp. $\Omega = [\text{supp}(P_{\beta_0})]^{\mathbb{Z}}$) and hence Ω is a compact topological space with respect to the product topology. Thus we may speak of the support of the probability measure P.

Since in almost all of the following results, $-\Delta_{\alpha(\omega),\Lambda}$ and $\Xi_{\beta(\omega),\Lambda}$ can be treated on exactly the same footing, we now introduce the following unifying notation: First of all, we replace $\alpha(\omega)$ and $\beta(\omega)$ by $\gamma(\omega) = \{\gamma_j(\omega) \in \mathbb{R}\}_{j\in\mathbb{Z}}$ with γ_j, $j \in \mathbb{Z}$, i.i.d. random variables with compact support. Moreover, because of the above identification $\Omega = [\text{supp}(P_{\gamma_0})]^{\mathbb{Z}}$, any $\omega \in \Omega$ is given by $\omega = \prod_{j\in\mathbb{Z}} \omega_j$ and $\omega_j = \gamma_j(\omega)$, $j \in \mathbb{Z}$, in this representation. The operator H_ω in $L^2(\mathbb{R})$ then represents $-\Delta_{\omega,\Lambda}$ or $\Xi_{\omega,\Lambda}$ (i.e., $\omega_j = \gamma_j(\omega)$ now plays the role of $\alpha_j(\omega)$ or $\beta_j(\omega)$, $j \in \mathbb{Z}$). The corresponding deterministic operators $-\Delta_{\alpha,\Lambda}$ and $\Xi_{\beta,\Lambda}$ are in general represented by the symbol $H_{\xi,\Lambda}$.

Next let $\{T_j\}_{j\in\mathbb{Z}}$ be the shift operator in Ω defined by

$$(T_l\omega)_j = \omega_{j-l}, \qquad \omega \in \Omega, \quad j, l \in \mathbb{Z}, \tag{5.3.1}$$

such that

$$\gamma_j(T_l\omega) = \gamma_{j-l}(\omega) = \omega_{j-l}, \qquad \omega \in \Omega, \quad j, l \in \mathbb{Z}. \tag{5.3.2}$$

As in Sect. 5.2, $\{T_j\}_{j\in\mathbb{Z}}$ is a family of measure preserving, ergodic transformations. Moreover, let $\{U_j\}_{j\in\mathbb{Z}}$ denote the family of unitary translation operators in $L^2(\mathbb{R})$

$$(U_j g)(x) = g(x - ja), \qquad g \in L^2(\mathbb{R}), \quad j \in \mathbb{Z}. \tag{5.3.3}$$

As in Sect. 5.2, $\{U_j\}_{j\in\mathbb{Z}}$ is complete in the sense of Sect. 5.1 and

$$U_j H_\omega U_j^{-1} = H_{T_j\omega}, \qquad \omega \in \Omega, \quad j \in \mathbb{Z}. \tag{5.3.4}$$

Since the proof of these statements and of the analogs of Theorems 5.2.2 and 5.2.3 can be translated into the present situation word by word (some technicalities even become simpler since $G_k(0)$ is bounded in one dimension) we have

Theorem 5.3.1. *Let $\{H_\omega\}_{\omega\in\Omega}$ be defined as above. Then $\sigma(H_\omega)$, $\sigma_{\text{ess}}(H_\omega)$, $\sigma_{\text{c}}(H_\omega)$, $\sigma_{\text{ac}}(H_\omega)$, $\sigma_{\text{sc}}(H_\omega)$, and $\overline{\sigma_{\text{p}}(H_\omega)}$ all equal certain nonrandom sets Σ, Σ_{ess}, Σ_{c}, Σ_{ac}, Σ_{sc}, and Σ_{p} for P-a.e. $\omega \in \Omega$. Moreover, $\sigma_{\text{d}}(H_\omega) = \varnothing$ for P-a.e. $\omega \in \Omega$. For any $\tau \in \mathbb{R}$ there exists a subset $\Omega_\tau \subseteq \Omega$ with $P(\Omega_\tau) = 1$ such that τ is no eigenvalue of H_ω, $\omega \in \Omega_\tau$.*

PROOF. As mentioned above only the last assertion concerning the fact that any $\tau \in \mathbb{R}$ is P-a.s. no eigenvalue of H_ω needs a proof. But this holds since any eigenvalue of H_ω has multiplicity less than or equal to two. ∎

In order to state the analog of Theorem 5.2.2 we again introduce the concept of stochastic (resp. admissible) potentials. A sequence $\Phi(\omega) = \{\gamma_j(\omega) \in \mathbb{R}\}_{j\in\mathbb{Z}}$, $\omega \in \Omega$, with γ_j, $j \in \mathbb{Z}$, i.i.d. random variables and $\text{supp}(P_{\gamma_0})$ compact is called a stochastic potential. In contrast to Sect. 5.2 there is now no need to introduce the stochastic variables X_j, $j \in \mathbb{Z}$, since $\gamma_j(\omega) = 0$ is possible whenever $P(\gamma_j = 0) > 0$. The class $\mathscr{A}$ of admissible potentials then consists of elements

$\phi = \{\xi_j \in \operatorname{supp}(P_{\gamma_0})\}_{j \in \mathbb{Z}}$. The class $\mathscr{P}$ of all periodic admissible potentials is then given by all $\phi \in \mathscr{A}$ such that the corresponding sequence $\{\xi_j\}_{j \in \mathbb{Z}}$ satisfies

$$\xi_{j+L} = \xi_j, \qquad j \in \mathbb{Z}, \tag{5.3.5}$$

for some $L \in \mathbb{Z} - \{0\}$. For $\phi \in \mathscr{A}$, $H(\phi)$ denotes the Hamiltonian H_ω with $\gamma_j(\omega)$ replaced by ξ_j, $j \in \mathbb{Z}$ (i.e., $H(\phi) = H_{\xi,\Lambda}$). Then we get

Theorem 5.3.2. *Let $\Phi(\omega)$ be the stochastic potential as defined above. Then*

(i)
$$\sigma(H(\phi)) \subseteq \Sigma, \qquad \phi \in \mathscr{A}, \tag{5.3.6}$$

(ii)
$$\Sigma = \bigcup_{\phi \in \mathscr{A}} \sigma(H(\phi)) = \overline{\bigcup_{\phi \in \mathscr{P}} \sigma(H(\phi))}, \tag{5.3.7}$$

where $\Sigma = \sigma(H(\Phi(\omega)))$ for P-a.e. $\omega \in \Omega$.

As remarked before, one can follow the proof of Theorem 5.2.3 step by step. We also note that Theorem 5.3.2(i) above simply means

$$\sigma(H_\omega) \subseteq \Sigma, \qquad \omega \in \operatorname{supp}(P) \tag{5.3.8}$$

since $\omega \in \operatorname{supp}(P)$ implies that ϕ_ω defined as

$$\phi_\omega = \{\omega_j\}_{j \in \mathbb{Z}} \in \mathscr{A}, \qquad \omega = \prod_{j \in \mathbb{Z}} \omega_j, \tag{5.3.9}$$

is an admissible potential.

Next we state

Theorem 5.3.3. *Under the assumptions of Theorem 5.3.2 we get*

$$\Sigma = \bigcup_{\xi \in \operatorname{supp}(P_{\gamma_0})} \sigma(H_{\xi,\Lambda}). \tag{5.3.10}$$

Proof. Since $H_{\xi,\Lambda} = H(\phi)$ with $\phi = \{\xi_j = \xi \in \operatorname{supp}(P_{\gamma_0})\}_{j \in \mathbb{Z}}$ Theorem 5.3.2(ii) implies

$$\Sigma_0 \subseteq \Sigma, \tag{5.3.11}$$

where

$$\Sigma_0 = \bigcup_{\xi \in \operatorname{supp}(P_{\gamma_0})} \sigma(H_{\xi,\Lambda}). \tag{5.3.12}$$

Conversely, there is a $\phi = \{\xi_j \in \operatorname{supp}(P_{\gamma_0})\}_{j \in \mathbb{Z}} \in \mathscr{A}$ such that $\sigma(H(\phi)) = \Sigma$ (this is even true for P-a.e. $\omega = \{\xi_j\}_{j \in \mathbb{Z}} \in \Omega$). By Theorem 2.3.6 we know that if $(c, d) \cap \Sigma_0 = \varnothing$ then also

$$(c, d) \cap \Sigma = (c, d) \cap \sigma(H(\phi)) = \varnothing. \tag{5.3.13}$$

Thus

$$\Sigma \subset \bar{\Sigma}_0. \tag{5.3.14}$$

In the rest of the proof we show that Σ_0 is closed implying $\Sigma = \Sigma_0$. By Theorems

2.3.3 and 3.6 we have

$$\sigma(H_{\gamma,\Lambda}) = \bigcup_{m=1}^{\infty} [a_m^{\gamma,\Lambda}, b_m^{\gamma,\Lambda}], \qquad a_m^{\gamma,\Lambda} < b_m^{\gamma,\Lambda} \le a_{m+1}^{\gamma,\Lambda}, \quad \gamma \in \mathbb{R}, \quad m \in \mathbb{N}. \tag{5.3.15}$$

Thus

$$B_m = \bigcup_{\xi \in \operatorname{supp}(P_{\gamma_0})} [a_m^{\xi,\Lambda}, b_m^{\xi,\Lambda}] \subseteq [a_m^{\xi_-,\Lambda}, b_m^{\xi_+,\Lambda}] \tag{5.3.16}$$

for some $\xi_\pm \in \operatorname{supp}(P_{\gamma_0})$. Here we used the compactness of $\operatorname{supp}(P_{\gamma_0})$ and the continuity of $a_m^{\xi,\Lambda}$, $b_m^{\xi,\Lambda}$, $m \in \mathbb{N}$, with respect to $\xi \in \mathbb{R}$. Let $\{x_n\}_{n\in\mathbb{N}} \subset B_m$ be a Cauchy sequence. Then there is a $x_0 \in [a_m^{\xi_-,\Lambda}, b_m^{\xi_+,\Lambda}]$ such that $\lim_{n\to\infty} x_n = x_0$ and $x_n \in [a_m^{\xi_n,\Lambda}, b_m^{\xi_n,\Lambda}]$ for some $\{\xi_n\}_{n\in\mathbb{N}} \subseteq \operatorname{supp}(P_{\gamma_0})$. By the compactness of $\operatorname{supp}(P_{\gamma_0})$ there is a subsequence $\{\tilde{\xi}_n\}_{n\in\mathbb{N}}$ of $\{\xi_n\}_{n\in\mathbb{N}}$ such that $\lim_{n\to\infty} \tilde{\xi}_n = \xi_0 \in \operatorname{supp}(P_{\gamma_0})$. Because of $a_m^{\xi_n,\Lambda} \le x_n \le b_m^{\xi_n,\Lambda}$, and the above-mentioned continuity with respect to ξ, we infer $a_m^{\xi_0,\Lambda} \le x_0 \le b_m^{\xi_0,\Lambda}$. Thus $x_0 \in B_m$ and hence B_m, $m \in \mathbb{N}$, are closed. Taking into account the constraints on $a_m^{\xi,\Lambda}$, $b_m^{\xi,\Lambda}$, $m \in \mathbb{N}$, as described in Theorems 2.3.3 and 3.6 we finally infer that $\Sigma_0 = \bigcup_{m=1}^{\infty} B_m$ is closed. ∎

Corollary 5.3.4. *Assume the hypotheses of Theorem* 5.3.2 *and denote by* $\mu = \inf[\operatorname{supp}(P_{\gamma_0})]$, $\nu = \sup[\operatorname{supp}(P_{\gamma_0})]$. *Then we have*

(i)
$$\Sigma = \bigcup_{m=1}^{\infty} [a_m, b_m], \qquad a_m < b_m \le a_{m+1}, \quad a_m, b_m \xrightarrow[m\to\infty]{} \infty. \tag{5.3.17}$$

(ii) *If* $\mu \ge 0$, *then*

$$\Sigma = \sigma(H_{\mu,\Lambda}). \tag{5.3.18}$$

(iii) $\sigma(H_\omega)$ *has infinitely many open gaps for* P-a.e. $\omega \in \Omega$ *unless* $0 \in \operatorname{supp}(P_{\gamma_0})$. *If* $0 \in \operatorname{supp}(P_{\gamma_0})$ *then*

$$[0, \infty) \subseteq \Sigma \tag{5.3.19}$$

and there are at most finitely many gaps in $(-\infty, 0)$.

(iv) *Assume* $\operatorname{supp}(P_{\gamma_0}) = [\mu, \nu]$ (*or* $b_1^{\mu,\Lambda} \ge a_1^{\nu,\Lambda}$). *If* $\nu \le 0$ *then*

$$\Sigma = [a_1^{\mu,\Lambda}, a_1^{\nu,\Lambda}] \cup \sigma(-\Delta_{\nu,\Lambda}) \tag{5.3.20}$$

in the case where $H_\omega = -\Delta_{\omega,\Lambda}$ *represents* δ-*interactions. If* $\nu \le -a$

$$\Sigma = \sigma(\Xi_{\nu,\Lambda}) \tag{5.3.21}$$

in the case where $H_\omega = \Xi_{\omega,\Lambda}$ *represents* δ'-*interactions.*

PROOF. (i) follows from the fact that

$$\Sigma = \bigcup_{\xi\in\operatorname{supp}(P_{\gamma_0})} \bigcup_{m=1}^{\infty} [a_m^{\xi,\Lambda}, b_m^{\xi,\Lambda}] \tag{5.3.22}$$

with $a_m^{\xi,\Lambda}, b_m^{\xi,\Lambda} \xrightarrow[m\to\infty]{} \infty$.

(ii)–(iv) follows from (5.3.10) and the monotonicity statements in (2.3.39) and (3.49). ∎

Finally, we prove the *Saxon and Hutner conjecture* for random systems.

Theorem 5.3.5. *Assume the hypotheses of Theorem* 5.3.2. *Let* $\Gamma \subset \mathbb{R}$ *be open and* $\Gamma \subseteq \bigcap_{\lambda \in \operatorname{supp}(P_{\gamma_0})} \rho(H_{\lambda,\Lambda})$. *Then*

$$\Gamma \cap \Sigma = \varnothing. \tag{5.3.23}$$

PROOF. We only need to combine Theorems 2.3.6 and 5.3.3. ■

Notes

Section III.5.1

The entire material is taken from work of Kirsch and Martinelli [286], [287]. Their results extend earlier results by Pastur [368] and Kunz and Souillard [309] for the discrete Schrödinger operator. Another approach for the non-randomness of the spectrum of ergodic Schrödinger operators appeared in [170], [311]. For an extensive survey on random Schrödinger operators, cf. [119] and [128], Ch. 9.

Section III.5.2

This section is based on work of Albeverio, Høegh-Krohn, Kirsch, and Martinelli [30], [287], [288], [289]. Our presentation closely follows [20]. We also emphasize the fact that every result in this section stated for the three-dimensional model has a word-by-word translation into the corresponding two-dimensional system.

A discussion of point interactions on random manifolds is given in [14]. Applications to statistical mechanics of polymers and quantum field theory appeared in [13], [14].

For a general study of the Laplacian with boundary conditions on small, randomly distributed spheres, cf. [181], [182], [183] and the literature therein. Multiple scattering of waves by randomly distributed point scatterers has been discussed in [186].

Some applications in quantum chemistry appeared in [80].

Section III.5.3

In the case of δ-interactions the material is based on work of Kirsch and Martinelli [286], [287], [288], [289], in the case of δ'-interactions it is based on [205] and [206]. Our presentation closely follows [206] (cf. also [20]). The general formulation of the Saxon and Hutner conjecture in Theorem 5.3.5 is due to [206]. Earlier results in the case of δ-interactions in [286], [287], [288], [289] used additional restrictions on the sign of the coupling constants (i.e., $\lambda_j \geq 0$ or $\lambda_j \leq 0, j \in \mathbb{Z}$). A result essentially implying Theorem 3.5.3 in the case of δ-interactions was given in [165], [168]. As shown in [206], the results of this section can be extended to the case where $\{\gamma_j\}_{j \in \mathbb{Z}}$ is an ergodic (i.e., metrically transitive) stochastic process with $|\gamma_j(\omega)| \leq C, j \in \mathbb{Z}, \omega \in \Omega$. Theorem 5.3.1 immediately extends to this situation. The rest of this section also extends to this situation provided $\operatorname{supp}(P) = \Omega = [\operatorname{supp}(P_{\gamma_0})]^{\mathbb{Z}}$ (assuming $\operatorname{supp}(P_{\gamma_0})$ to be compact). The last hypothesis is, e.g., satisfied by a stationary Markov process $\{\gamma_j\}_{j\in\mathbb{Z}}$ with transition function $p(x, A) > 0$ for all $x \in \operatorname{supp}(P_{\gamma_0})$, $A \subset \operatorname{supp}(P_{\gamma_0})$, A open. Another extension we would like to mention is the possibility of including random deviations from lattice positions as discussed in [289].

There has been considerable interest in the problem of determining the nature of the spectrum of H_ω. In the case of δ-interactions, P-a.s. exponential localization of the spectrum (i.e., the existence of a complete set of exponentially decaying eigenfunctions in $L^2(\mathbb{R})$) has been proven [143], [144] under the assumptions that $\{\alpha_j\}_{j\in\mathbb{Z}}$ are i.i.d. random variables with a density r satisfying $\|r\|_\infty < \infty$ and that

$$p = \sup\{x > 0 \,|\, E(|\cdot|^x) < \infty\} > 0.$$

For earlier results in this direction cf., e.g., [217]. Applying the methods of [144] these results are expected to extend to the δ'-case.

Another problem that has been studied intensively was the nature of the spectrum of random δ-interactions in the presence of an external electric field as a function of the field strength F. Then the Hamiltonian in $L^2(\mathbb{R})$ is given by

$$H_\omega(F) = -\Delta_{\alpha(\omega),\Lambda} + Fx, \qquad F \le 0.$$

As proven in [143], [144] under the assumptions of the preceding paragraph, for $F_1 < F < 0$, $H_\omega(F)$ has P-a.s. a pure point spectrum with power decaying eigenfunctions. For sufficiently strong fields, $F < F_2 < F_1$ and $p > 2$, $H_\omega(F)$ has P-a.s. a purely continuous spectrum. This transition from a pure point spectrum (for sufficiently weak electric fields) to a purely continuous spectrum (for sufficiently strong electric fields) is quite remarkable, since for one-dimensional Schrödinger operators with $\sum_{j\in\mathbb{Z}} \alpha_j(\omega)\delta(x - ja)$ replaced by a sufficiently smooth $V_\omega(x)$, the system does not exhibit localization at all. In fact, in this case the spectrum turns out to be purely absolutely continuous [75], [118], [119]. Numerical studies of this transition mentioned above have been reported in [78], [382], and [451]. A numerical study of resonances in such systems appeared in [73], [74], [78].

Finally, we note that there exists a vast number of papers in the physics literature dealing with random δ-interactions. Mainly two cases have been studied in great detail: *Random alloys* (i.e., the systems described in this section where the positions form a deterministic lattice Λ and the coupling constants are random variables) or *liquid metals* (i.e., deterministic coupling constants but random positions). Random alloys are treated, e.g., in [6], [116a], [230], [236], [241], [254], [255], [256], [257], [258], [259], [282], [303], [361], [408], [476] [492] and liquids in [66], [91], [92], [102], [103], [104], [105], [163], [189], [236], [240], [273], [291], [319], [330], [336], [361], [373], [375], [393], [476], [477], [491]. For a critical survey of some of these results, cf. [174] (see also [164], [173]). Mathematical results on the density of states associated with these two types of systems can be found in [163], [164], [222], [223], and [268].

Multiple scattering of waves by randomly distributed point scatterers appeared, e.g., in [40], [63], [64], [65], [234], [235], [337], [337a], and [403].

APPENDICES

APPENDIX A

Self-Adjoint Extensions of Symmetric Operators

Assume $\dot{A}$ to be a densely defined, closed, symmetric operator in some Hilbert space $\mathscr{H}$ with deficiency indices (1, 1). If

$$\dot{A}^*\phi(z) = z\phi(z), \qquad \phi(z) \in \mathscr{D}(\dot{A}^*), \quad z \in \mathbb{C} - \mathbb{R}, \tag{A.1}$$

we have

Theorem A.1. *All self-adjoint extensions A_θ of $\dot{A}$ may be parametrized by a real parameter $\theta \in [0, 2\pi)$ where*

$$\begin{gathered} \mathscr{D}(A_\theta) = \{g + c\phi_+ + ce^{i\theta}\phi_- | g \in \mathscr{D}(\dot{A}), c \in \mathbb{C}\}, \\ A_\theta(g + c\phi_+ + ce^{i\theta}\phi_-) = \dot{A}g + ic\phi_+ - ice^{i\theta}\phi_-, \qquad 0 \leq \theta < 2\pi, \end{gathered} \tag{A.2}$$

and

$$\phi_\pm = \phi(\pm i), \qquad \|\phi_+\| = \|\phi_-\|. \tag{A.3}$$

Concerning resolvents of self-adjoint extensions of $\dot{A}$ we state

Theorem A.2 (Krein's Formula). *Let B and C denote any self-adjoint extensions of $\dot{A}$. Then we have that*

$$(B - z)^{-1} - (C - z)^{-1} = \lambda(z)(\phi(\bar{z}), \cdot)\phi(z), \qquad z \in \rho(B) \cap \rho(C), \tag{A.4}$$

where $\lambda(z) \neq 0$ for $z \in \rho(B) \cap \rho(C)$ and λ and ϕ may be chosen to be analytic in $z \in \rho(B) \cap \rho(A)$. In fact, $\phi(z)$ may be defined as

$$\phi(z) = \phi(z_0) + (z - z_0)(C - z)^{-1}\phi(z_0), \qquad z \in \rho(C), \tag{A.5}$$

where $\phi(z_0)$, $z_0 \in \mathbb{C} - \mathbb{R}$, *is a solution of* (A.1) *for* $z = z_0$ *and* $\lambda(z)$ *satisfies*

$$\lambda(z)^{-1} = \lambda(z')^{-1} - (z - z')(\phi(\bar{z}), \phi(z')), \qquad z, z' \in \rho(B) \cap \rho(C), \quad \text{(A.6)}$$

if $\phi(z)$ *is chosen according to* (A.5).

Next we turn to the general case and assume that $\dot{A}$ is a densely defined, closed symmetric operator in $\mathscr{H}$ with deficiency indices (N, N), $N \in \mathbb{N}$. Let B and C be two self-adjoint extensions of $\dot{A}$ and denote by $\mathring{A}$ the maximal common part of B and C (i.e., $\mathring{A}$ obeys $\mathring{A} \subseteq B$, $\mathring{A} \subseteq C$ and $\mathring{A}$ extends any operator A' that fulfills $A' \subseteq B$, $A' \subseteq C$). Let M, $0 < M \leq N$, be the deficiency indices of $\mathring{A}$ and let $\{\phi_1(z), \ldots, \phi_M(z)\}$ span the corresponding deficiency subspace of $\mathring{A}$, i.e.,

$$\mathring{A}^* \phi_m(z) = z\phi_m(z), \qquad \phi_m(z) \in \mathscr{D}(\mathring{A}^*), \quad m = , \ldots, M, \quad z \in \mathbb{C} - \mathbb{R}, \quad \text{(A.7)}$$

and $\{\phi_1(z), \ldots, \phi_M(z)\}$ are linearly independent. Then the analog of Theorem A.2 reads

Theorem A.3 (Krein's Formula for Deficiency Indices $N > 1$). *Let* B, C, $\mathring{A}$, *and* $\dot{A}$ *be as above. Then*

$$(B - z)^{-1} - (C - z)^{-1} = \sum_{m,n=1}^{M} \lambda_{mn}(z)(\phi_n(\bar{z}), \cdot)\phi_m(z), \qquad z \in \rho(B) \cap \rho(C), \quad \text{(A.8)}$$

where the matrix $\lambda(z)$ *is nonsingular for* $z \in \rho(B) \cap \rho(C)$ *and* $\lambda_{mn}(z)$ *and* $\phi_m(z)$, $m, n = 1, \ldots, M$, *may be chosen to be analytic in* $z \in \rho(B) \cap \rho(C)$. *In fact,* $\phi_m(z)$ *may be defined as*

$$\phi_m(z) = \phi_m(z_0) + (z - z_0)(C - z)^{-1}\phi_m(z_0), \qquad m = 1, \ldots, M, \quad z \in \rho(C), \quad \text{(A.9)}$$

where $\phi_m(z_0)$, $m = 1, \ldots, M$, $z_0 \in \mathbb{C} - \mathbb{R}$, *are linearly independent solutions of* (A.7) *for* $z = z_0$ *and the matrix* $\lambda(z)$ *satisfies*

$$[\lambda(z)]_{mn}^{-1} = [\lambda(z')]_{mn}^{-1} - (z - z')(\phi_n(\bar{z}), \phi_m(z')), \qquad m, n = 1, \ldots, M,$$
$$z, z' \in \rho(B) \cap \rho(C), \quad \text{(A.10)}$$

if the $\phi_m(z)$, $m = 1, \ldots, M$, *are defined according to* (A.9).

In general, we have

$$(B - z)^{-1} - (C - z)^{-1} = \sum_{m,n=1}^{N} \tilde{\lambda}_{mn}(z)(\tilde{\phi}_n(\bar{z}), \cdot)\tilde{\phi}_m(z), \quad z \in \rho(B) \cap \rho(C), \quad \text{(A.11)}$$

where now $\tilde{\phi}_m(z)$, $m = 1, \ldots, N$, are linearly independent solutions of

$$\dot{A}^* \tilde{\phi}_m(z) = z\tilde{\phi}_m(z), \qquad \tilde{\phi}_m(z) \in \mathscr{D}(\dot{A}^*), \quad m = 1, \ldots, N, \quad z \in \mathbb{C} - \mathbb{R}, \quad \text{(A.12)}$$

and, in general, $\det \tilde{\lambda}(z) \equiv 0$.

Notes

Self-adjoint extensions of densely defined, symmetric operators are discussed in various monographs ([8], Ch. VII, [158], Ch. XII.4, [353], Ch. IV.14, [389], Ch. X.1, [494], Ch. 8; see also [38], [267], [267a], [299], [356], [398], [399], [470], [471].

APPENDIX B

Spectral Properties of Hamiltonians Defined as Quadratic Forms

Let H_0 be a self-adjoint, semibounded operator in some separable (complex) Hilbert space $\mathscr{H}$. We denote by $\mathscr{B}(\mathscr{H})$ and $\mathscr{B}_\infty(\mathscr{H})$ the spaces of bounded and compact operators in $\mathscr{H}$, respectively, and by $\mathscr{B}_p(\mathscr{H})$, $p \geq 1$, the set of compact operators whose singular values are in l^p. Assume the condition

(I) E_j, F_j, $j = 1, \ldots, N$, $N \in \mathbb{N}$, are closed operators in $\mathscr{H}$ which are infinitesimally bounded with respect to $|H_0|^{1/2}$.

We then define in $\mathscr{H}$

$$H = H_0 \dotplus \sum_{j=1}^{N} E_j^* F_j \tag{B.1}$$

by the method of forms ([283], Ch. VI, [434], Ch. II) (in general H is not self-adjoint) and introduce in $\mathscr{H}^N = \bigoplus_{j=1}^N \mathscr{H}$ the family of bounded operators $K(k) \in \mathscr{B}(\mathscr{H}^N)$

$$K(k)\colon \mathscr{H}^N \to \mathscr{H}^N, \qquad (K(k)(g_1, \ldots, g_N))_j = \sum_{j'=1}^{N} K_{jj'}(k) g_{j'},$$
$$g_j \in \mathscr{H}, \quad j = 1, \ldots, N, \tag{B.2}$$

here

$$K_{jj'}(k) = F_j(H_0 - k^2)^{-1} E_{j'}^*, \quad k^2 \in \rho(H_0), \quad \operatorname{Im} k > 0, \quad j, j' = 1, \ldots, N. \tag{B.3}$$

(If no confusion arises we always identify operators of the type $(H_0 - k^2)^{-1} E_j^*$ and $[E_j(H_0 - \bar{k}^2)^{-1}]^*$, etc.) Next we assume

(II) $K_{jj'}(k) \in \mathscr{B}_\infty(\mathscr{H})$, $\quad j, j' = 1, \ldots, N, \quad$ for all $\quad \operatorname{Im} k > 0, \quad k^2 \in \rho(H_0)$.

Then we have

Theorem B.1.

(a) *Suppose condition* (I) *holds. Then*

$$(H - k^2)^{-1} = (H_0 - k^2)^{-1} - \sum_{j=1}^{N} (H_0 - k^2)^{-1} E_j^* F_j (H_0 - k^2)^{-1},$$

$$k^2 \in \rho(H) \cap \rho(H_0). \quad \text{(B.4)}$$

(b) *Assume hypothesis* (I) *and* (II). *Then*

$$(H - k^2)^{-1} = (H_0 - k^2)^{-1} - \sum_{j,j'=1}^{N} (H_0 - k^2)^{-1} E_j^* [1 + K(k)]_{jj'}^{-1} F_{j'} (H_0 - k^2)^{-1},$$

$$\operatorname{Im} k > 0, \quad k^2 \in \rho(H) \cap \rho(H_0). \quad \text{(B.5)}$$

and

$$\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0). \quad \text{(B.6)}$$

(c) *Assume conditions* (I) *and* (II) *and let* $E_0 = k_0^2 \in \rho(H_0)$, $\operatorname{Im} k_0 > 0$. *Then* H *has the eigenvalue* E_0 *with geometric multiplicity* M *if and only if* $K(k_0)$ *has the eigenvalue* -1 *with the same geometric multiplicity* M. *In particular, if* $K(k_0)\Phi_0 = -\Phi_0$, $\Phi_0 = (\phi_{01}, \ldots, \phi_{0N}) \in \mathscr{H}^N$ *then* $\psi_0 = \sum_{j=1}^{N} (H_0 - k_0^2)^{-1} E_j^* \phi_{0j}$ *fulfills* $\psi_0 \in \mathscr{D}(H)$, $H\psi_0 = E_0\psi_0$. *Conversely, if* $H\tilde{\psi}_0 = E_0\tilde{\psi}_0$, $\tilde{\psi}_0 \in \mathscr{D}(H)$, *then* $\tilde{\Phi}_0 = (\tilde{\phi}_{01}, \ldots, \tilde{\phi}_{0N}) \in \mathscr{H}^N$, $\tilde{\phi}_{0j} = -F_j\tilde{\psi}_0$, $j = 1, \ldots, N$, *fulfills* $K(k_0)\tilde{\Phi}_0 = -\tilde{\Phi}_0$ *and* $\tilde{\psi}_0 = \sum_{j=1}^{N} (H_0 - k_0^2)^{-1} E_j^* \tilde{\phi}_{0j}$.

In order to treat resonances of H we need, in addition, hypothesis

(III) Let $\Omega \subseteq \mathbb{C}$ be open and connected, $\Omega \supseteq \{k \in \mathbb{C} \mid \operatorname{Im} k > 0, k^2 \in \rho(H_0)\}$, $k_0 \in \Omega$ for some k_0 with $\operatorname{Im} k_0 < 0$. Assume that $K\colon \Omega \to \mathscr{B}_\infty(\mathscr{H}^N)$.

By Theorem B.1(c) there exists a one-to-one correspondence between eigenvalues $E_1 = k_1^2$, $\operatorname{Im} k_1 > 0$, $k_1 \in \Omega$, of H and the eigenvalue -1 of $K(k_1)$. For *resonances* we introduce the following definition:

Assume hypotheses (I) and (II). Then $k_2 \in \Omega$, $\operatorname{Im} k_2 < 0$, is called a resonance of H if and only if $K(k_2)$ has the eigenvalue -1.

For a discussion of multiplicities of eigenvalues and resonances we add assumption

(IV) In addition to condition (III) assume that K is (norm) analytic in Ω and that $K\colon \Omega \to \mathscr{B}_p(\mathscr{H}^N)$ for some $p \in \mathbb{N}$.

Theorem B.2. *Assume hypotheses* (I) *and* (IV). *Then, if for some* $k_0 \in \Omega$, $K(k_0)$ *has an eigenvalue* -1, $[1 + K(k)]^{-1}$ *has a norm convergent Laurent expansion around* $k = k_0$, *viz.*

$$[1 + K(k)]^{-1} = \sum_{m=-m_0}^{\infty} K_m (k - k_0)^m \quad \text{for some} \quad m_0 \in \mathbb{N} \cup \{0\}. \quad \text{(B.7)}$$

Here $K_m \in \mathscr{B}(\mathscr{H}^N)$ *for each* $m \geq -m_0$ *and for* $-m_0 \leq m \leq -1$, K_m *is of finite rank. Moreover,* $-1 \in \sigma(K(k_0))$ *if and only if* $\det_p[1 + K(k_0)] = 0$ *and the geometric multiplicity of the eigenvalue* -1 *of* $K(k_0)$ *coincides with the multiplicity of the zero of the (modified) Fredholm determinant* $\det_p[1 + K(k)]$ *at* $k = k_0$ *if and only if* $m_0 = 1$. *In particular, if* H *is self-adjoint and* $k_0 \in \Omega$, $\operatorname{Im} k_0 > 0$, *then* $m_0 = 1$.

That m_0 need not be one (e.g., if resonances collide) has been discussed in [365] and [385]. In fact, if $m_0 > 1$ then $\nu(k_0)$, the order of the zero of $\det_p[1 + K(k)]$ at $k = k_0$, strictly dominates the geometric multiplicity of the eigenvalue -1 of $K(k_0)$. (In general, $\nu(k_0) \geq m_0$) [262]. On the other hand, $[1 + K(k)]^{-1}$ has a simple pole at $k = k_0$ if and only if $[1 + K(k_0) + (k - k_0)K'(k_0)]^{-1}$ has a simple pole at $k = k_0$. In addition, if the geometric and algebraic multiplicity of the eigenvalue -1 of $K(k_0)$ coincide, then $[1 + K(k)]^{-1}$ has a simple pole at $k = k_0$ if and only if $P(k_0)K'(k_0)$ (or equivalently if $K'(k_0)$) is injective on $\operatorname{Ker}[1 + K(k_0)]$ [262]. (Here $P(k_0) = -(2\pi i)^{-1} \oint_{|z+1|=\varepsilon} dz [K(k_0) - z]^{-1}$, $\varepsilon > 0$ small enough, denotes the projection onto the algebraic eigenspace of $K(k_0)$ to the eigenvalue -1 and $\operatorname{Ker}[T]$ denotes the kernel of some $T \in \mathscr{B}(\mathscr{H}^N)$.)

Given hypotheses (I) and (IV) we therefore define the multiplicity of a resonance $k_0 \in \Omega$, $\operatorname{Im} k_0 < 0$, of H to be the multiplicity of the zero of the (modified) Fredholm determinant $\det_p[1 + K(k)]$ at $k = k_0$.

Finally, we discuss perturbations of eigenvalues and resonances and introduce condition

(V) Let $\Lambda \subseteq \mathbb{C}$ be open and connected and suppose $E_{j,\lambda}$, $F_{j,\lambda}$, $j = 1, \ldots, N$, fulfill hypothesis (I) for all $\lambda \in \Lambda$. Moreover, assume $K_{jj',\lambda}(k) = F_{j,\lambda}(H_0 - k^2)^{-1} E^*_{j',\lambda}$, $j, j' = 1, \ldots, N$, to be (norm) analytic in $\Omega \times \Lambda$, and for some $p \in \mathbb{N}$, $K_{jj',\lambda}(k) \in \mathscr{B}_p(\mathscr{H})$, $j, j' = 1, \ldots, N$, for all $(k, \lambda) \in \Omega \times \Lambda$.

In analogy to (B.1) we then define

$$H_\lambda = H_0 \dot{+} \sum_{j=1}^{N} E^*_{j,\lambda} F_{j,\lambda}, \qquad \lambda \in \Lambda. \tag{B.8}$$

It turns out that if $k_0 \in \Omega$ corresponds to a bound state ($\operatorname{Im} k_0 > 0$) or to a resonance ($\operatorname{Im} k_0 < 0$) of H_{λ_0} for some fixed $\lambda_0 \in \Lambda$ then, for $|\lambda - \lambda_0|$ small enough, H_λ has bound states (resp. resonances) $k(\lambda) \in \Omega$ with $k(\lambda) = k_0 + o(\lambda - \lambda_0)$. The functions $k(\lambda)$ are given by solutions of $\det_p[1 + K_\lambda(k)] = 0$ near (k_0, λ_0). More precisely, we have

Theorem B.3. *Assume hypothesis* (V). *If for some* $(k_0, \lambda_0) \in \Omega \times \Lambda$, $K_{\lambda_0}(k_0)$ *has an eigenvalue* -1 *such that the multiplicity of the zero of* $\det_p[1 + K_{\lambda_0}(k)]$ *at* $k = k_0$ *equals* M *then, for* $|\lambda - \lambda_0|$ *small enough, there exist* M *(not necessarily distinct) functions* $k_l(\lambda) \in \Omega$, $l = 1, \ldots, m$, *which are all the solutions of* $\det_p[1 + K_\lambda(k)] = 0$ *for* (k, λ) *near* (k_0, λ_0). *They are given* *by convergent Puiseux expansions near $\lambda = \lambda_0$, i.e., there are functions h_l analytic near $\lambda = \lambda_0$, $h_l(0) = 0$, $l = 1, \ldots, m$, such that*

$$\begin{aligned} k_l(\lambda) &= k_0 + h_l((\lambda - \lambda_0)^{1/m_l}) \\ &= k_0 + \sum_{r=1}^{\infty} a_{l,r}(\lambda - \lambda_0)^{r/m_l}, \quad m_l \geq 1,\ l = 1, \ldots, m,\ \sum_{l=1}^{m} m_l = M. \end{aligned} \tag{B.9}$$

If, e.g., k_0 corresponds to a simple bound state or resonance of H_{λ_0} (i.e., if $M = 1$), then $k(\lambda)$ is analytic in λ near $\lambda = \lambda_0$, viz.

$$k(\lambda) \underset{\lambda \to \lambda_0}{=} k_0 + k_1(\lambda - \lambda_0) + O((\lambda - \lambda_0)^2),$$

$$k_1 = -\frac{\left(\tilde{\Phi}_0, \left[\dfrac{\partial}{\partial \lambda} K_\lambda(k_0)\right]\Big|_{\lambda=\lambda_0} \Phi_0\right)}{\left(\tilde{\Phi}_0, \left[\dfrac{\partial}{\partial k} K_{\lambda_0}(k)\right]\Big|_{k=k_0} \Phi_0\right)}, \tag{B.10}$$

where

$$K_{\lambda_0}(k_0)\Phi_0 = -\Phi_0, \qquad K_{\lambda_0}(k_0)^*\tilde{\Phi}_0 = -\tilde{\Phi}_0, \quad \Phi_0, \tilde{\Phi} \in \mathscr{H}^N. \tag{B.11}$$

If Im $k_0 > 0$, $\lambda_0 \in \Lambda \cap \mathbb{R}$, *and H_λ is self-adjoint for λ in a real neighborhood of λ_0, the additional constraint $E_l(\lambda) = k_l(\lambda)^2 < 0$, $l = 1, \ldots, m$, for $\lambda \in \mathbb{R}$, $|\lambda - \lambda_0|$ small enough, in fact leads to $m_l = 1$, i.e., $k_l(\lambda)$, $l = 1, \ldots, m$, are analytic near $\lambda = \lambda_0$ (Rellich's theorem).*

We note that $(\tilde{\Phi}_0, \Phi_0) \neq 0$ and $(\tilde{\Phi}_0, [(\partial/\partial k)K_{\lambda_0}(k)]|_{k=k_0}\Phi_0) \neq 0$ by the remarks following Theorem B.2 since $M = 1$.

Finally, we note a general theorem concerning Puiseux series, part (b) of which is a part of Rellich's theorem.

Lemma B.4. *Let h: $U \to \mathbb{C}$, $U \subseteq \mathbb{C}$, a complex neighborhood of zero, be an analytic function, let $r \in \mathbb{N}$ and consider the multivalued function*

$$g(z) = h(z^{1/r}). \tag{B.12}$$

(a) *If $g(z) \in \mathbb{R}$ for all $z > 0$ sufficiently small for all the r branches of g (i.e., by taking all the r r*th *roots $z^{1/r}$ in the definition of g), then $r = 1$ or $r = 2$.*
(b) *If $g(z) \in \mathbb{R}$ for all $z \in \mathbb{R}$ sufficiently small for all the r branches of g, then $r = 1$ and g is analytic in U.*

Remark. The constraint $g(z) \in \mathbb{R}$ for $z > 0$ or $z \in \mathbb{R}$ can be replaced by $g(z) \in \alpha\mathbb{R}$ for $z \in \{\beta x \in \mathbb{C} | x > 0\}$ or $z \in \beta\mathbb{R}$ for arbitrary $\alpha, \beta \in \mathbb{C} - \{0\}$.

We have frequently been using a formula which is related to the so-called Weinstein–Aronszajn determinant

Lemma B.5. *Let $\mathscr{H}$ be a separable (complex) Hilbert space, let A be a closed operator in $\mathscr{H}$ and $\phi_j, \psi_j \in \mathscr{H}, j = 1, \ldots, N$. Then*

$$\left[A + \sum_{j=1}^{N} (\phi_j, \cdot)\psi_j - z\right]^{-1}$$

$$= (A - z)^{-1} - \sum_{j,j'=1}^{N} [M(z)]_{jj'}^{-1}([(A - z)^{-1}]^* \phi_{j'}, \cdot)(A - z)^{-1}\psi_j,$$

$$z \in \rho(A), \quad \det[M(z)] \neq 0, \quad \text{(B.13)}$$

where

$$M(z)_{jj'} = \delta_{jj'} + (\phi_j, (A - z)^{-1}\psi_{j'}). \quad \text{(B.14)}$$

Finally, we recall Sobolev's inequality.

Lemma B.6. *Let $0 < \lambda < n, n \in \mathbb{N}$, and suppose that $g \in L^p(\mathbb{R}^n)$, $h \in L^q(\mathbb{R}^n)$ with $p^{-1} + q^{-1} + \lambda n^{-1} = 2$ and $1 < p, q < \infty$. Then*

$$\int_{\mathbb{R}^{2n}} d^n x \, d^n x' \, |g(x)| \, |h(x')| \, |x - x'|^{-\lambda} \leq C(p, q, \lambda, n) \|g\|_p \|h\|_q. \quad \text{(B.15)}$$

Notes

The entire material is taken from [21] and [200]. Theorem B.1 in the case $N = 1$ appeared in [302] (note that H_0 need not be semibounded) and has been widely used in quantum mechanics [391], [434]. For $N = 2$ it first appeared in [295] and [297] and for general $N \in \mathbb{N}$ in [245] and [250] in the context of the multiple well problem.

Theorem B.2 is based on [262] and extends results in [357].

Theorem B.3 for $N = 1$ first appeared in [26] and has been abstracted in [200]. The proof given in [200] directly extends to the case $N > 1$.

For a discussion of resonances in the context of abstract analytic scattering theory see also [271].

Fredholm determinants are reviewed in [436], [438].

The first part of Theorem B.4 has been used in [386], while the second part enters in a crucial way in the proof of Rellich's theorem (see, e.g., [391], Theorem XII.3).

Lemma B.6 can be found, e.g., in [434], p. 12 and [389], p. 31.

APPENDIX C

Schrödinger Operators with Interactions Concentrated Around Infinitely Many Centers

We first consider Schrödinger operators H in $L^2(\mathbb{R}^n)$, $n \in \mathbb{N}$, with countably infinitely many local singularities of the potential which are uniformly separated from each other by a positive distance. Due to the local character of the interaction each singularity separately contributes to the total deficiency index of H:

Theorem C.1. *Let $J \subseteq \mathbb{Z} - \{0\}$ be a finite or countably infinite index set and $J_0 = J \cup \{0\}$. Assume*

(i) *$\Sigma_j \subset \mathbb{R}^n$, $n \in \mathbb{N}$ is a compact set of Lebesgue measure zero for all $j \in J$ and suppose $\Sigma_0 = \varnothing$.*
(ii) *$V_j \in L^2_{\text{loc}}(\mathbb{R}^n - \Sigma_j)$ are real-valued, $j \in J_0$, and*
 (a) *$\operatorname{supp} V_j$ compact for all $j \in J$, or*
 (b) *V_j are bounded from below on every compact subset of $\mathbb{R}^n - \Sigma_j$ for all $j \in J_0$.*
(iii) *For some $\varepsilon > 0$: $\operatorname{dist}(\{\operatorname{supp} V_j \cup \Sigma_j\}, \{\operatorname{supp} V_{j'} \cup \Sigma_{j'}\}) \geq \varepsilon$ for all $j, j' \in J_0, j \neq j'$.*
(iv) *$W \in L^\infty(\mathbb{R}^n)$ is real-valued.*

Define the minimal Schrödinger operators $\dot{H}_j$ and $\dot{H}$ in $L^2(\mathbb{R}^n)$ by

$$\dot{H}_j = -\Delta + V_j, \qquad \mathscr{D}(\dot{H}_j) = C_0^\infty(\mathbb{R}^n - \Sigma_j), \qquad j \in J_0, \tag{C.1}$$

$$\dot{H} = -\Delta + V + W, \qquad \mathscr{D}(\dot{H}) = C_0^\infty(\mathbb{R}^n - \Sigma), \tag{C.2}$$

where

$$V(x) = \sum_{j \in J_0} V_j(x), \qquad \Sigma = \bigcup_{j \in J_0} \Sigma_j. \tag{C.3}$$

If H_j (resp. H) denotes the closure of $\dot{H}_j$ (resp. $\dot{H}$) then

$$\operatorname{def}(H) = \sum_{j \in J_0} \operatorname{def}(H_j). \tag{C.4}$$

Since V_j, V, W are real-valued, H and H_j, $j \in J_0$, commute with complex conjugation and hence have equal deficiency indices.

In the text, we mainly use the above result with $V = V_j = W \equiv 0, \Sigma_j = \{y_j\}$, $\Sigma = Y, j \in J_0 \subseteq \mathbb{Z}$ (except in Ch. I.2 where $V_0 = W = 0$, $J = \{1\}$, $\Sigma_1 = \{y\}$, $V_1(x) = \gamma |x - y|^{-1}, \gamma \in \mathbb{R}, x, y \in \mathbb{R}^3, x \neq y$).

We now turn to the locality properties of certain self-adjoint extensions of symmetric operators.

Lemma C.2. *Let $N \subset \mathbb{R}^n$ be a closed set with zero Lebesgue measure, and let H be any self-adjoint extension of $-\Delta|_{C_0^\infty(\mathbb{R}^n - N)}$. Then H is* local *in the following sense: If $U \subseteq \mathbb{R}^n$ is open and $f \in \mathcal{D}(H)$ satisfies $f = 0$ in U, then also $Hf = 0$ in U.*

PROOF. Suppose first that $U \cap N = \varnothing$. Then

$$(Hf, g) = (f, -\Delta g) = 0 \tag{C.5}$$

for any $g \in C_0^\infty(\mathbb{R}^n)$ with $\operatorname{supp}(g) \subset U$. Hence

$$Hf|_U \perp C_0^\infty(U) \tag{C.6}$$

which implies that $Hf = 0$ in U. If $U \cap N \neq \varnothing$, we consider the open set $U - N$. By the above argument $Hf = 0$ in $U - N$, but N being of zero Lebesgue measure implies that $Hf = 0$ in U. ∎

To estimate the norm of countably infinite matrices, the following estimate is often useful.

Lemma C.3. *Let $\mathcal{H} = \bigoplus_{j=1}^\infty \mathcal{H}_j$, $\mathcal{H}_j$ being separable (complex) Hilbert spaces and consider the bounded operator $A = [A_{jj'}]_{j,j' \in \mathbb{N}}$. Then*

$$\|A\| \leq \|A\|_{\mathrm{H}}, \tag{C.7}$$

where the Holmgren bound $\|A\|_{\mathrm{H}}$ is defined by

$$\|A\|_{\mathrm{H}} = \left[\sup_{j' \in \mathbb{N}} \sum_{j=1}^\infty \|A_{jj'}\| \sup_{j \in \mathbb{N}} \sum_{j'=1}^\infty \|A_{jj'}\| \right]^{1/2}. \tag{C.8}$$

Note that $\|A\|_{\mathrm{H}}$ does not provide a norm as can be seen from the following counterexample. Let

$$A_n = \left[\begin{array}{c|c} \begin{matrix} 1 \,\ldots\ldots\, 1 \\ 2^{-1} \ldots\ldots 2^{-1} \\ 2^{-(n-1)} \ldots 2^{-(n-1)} \end{matrix} & 0 \\ \hline 0 & 0 \end{array} \right]. \tag{C.9}$$

Then

$$\|A_n + A_n^{\mathrm{T}}\|_{\mathrm{H}} = n + 2[1 - 2^{-n}], \quad \|A_n\|_{\mathrm{H}} = \|A_n^{\mathrm{T}}\|_{\mathrm{H}} = [2n(1 - 2^{-n})]^{1/2} \tag{C.10}$$

and hence the triangle inequality is violated for n sufficiently large. (Here A_n^{T} denotes the transposed matrix of A_n.)

Our next result generalizes (B.5) to the case where the total interaction is an infinite sum of potentials with nonoverlapping support. First, we introduce some notation: Let

$$\mathscr{H} = \bigoplus_{j=1}^{\infty} L^2(\mathbb{R}^3) \tag{C.11}$$

and define bounded operators

$$\begin{aligned} &A_k: \mathscr{H} \to L^2(\mathbb{R}^3), && A_k = \sum_{j=1}^{\infty} (u_j, \cdot)G_k, \\ &B_k: \mathscr{H} \to \mathscr{H}, && B_k = [u_j G_k v_{j'}]_{jj'} \in \mathbb{N}, \\ &C_k: L^2(\mathbb{R}^3) \to \mathscr{H}, && C_k = [(\overline{G_k}, \cdot)v_j]_{j \in \mathbb{N}}, \qquad \operatorname{Im} k > 0, \end{aligned} \tag{C.12}$$

where the potentials satisfy

$$\begin{aligned} &V_j \in R, \qquad \operatorname{supp} V_j \text{ compact}, \qquad \operatorname{supp} V_j \cap \operatorname{supp} V_{j'} = \varnothing, \\ &|V_j| \le V, \qquad V \in R, \quad j \ne j', \quad j, j' \in \mathbb{N}. \end{aligned} \tag{C.13}$$

Then we state

Theorem C.4. *Let V_j, $j \in \mathbb{N}$, be real-valued and satisfy* (C.13). *Then the self-adjoint operator*

$$H = -\Delta \dotplus \sum_{j=1}^{\infty} V_j \tag{C.14}$$

has the resolvent

$$(H - k^2)^{-1} = G_k - A_k[1 + B_k]^{-1} C_k, \qquad k^2 \in \rho(H), \quad \operatorname{Im} k > 0. \tag{C.15}$$

Next we study form perturbations of $-\Delta$ on $H^{2,2}(\mathbb{R}^n)$, $n \in \mathbb{N}$, in more detail. Let $Y = \{y_j\}_{j \in J}$, $J \subset \mathbb{Z}^n$, denote a discrete subset of $\mathbb{R}^n$ such that

$$\inf_{\substack{j,j' \in J \\ j \ne j'}} |y_j - y_{j'}| = d > 0, \qquad y_j, y_{j'} \in Y, \quad j, j' \in J. \tag{C.16}$$

Let $C_0 = \{x = (x^1, \ldots, x^n) \in \mathbb{R}^n | 2x^l \in (-1, 1], l = 1, \ldots, n\}$ denote the corresponding unit cell and define $C_j = C_0 + j, j \in \mathbb{Z}^n$. Assume q to be a symmetric form bounded with respect to the form of $-\Delta$ on $H^{2,2}(\mathbb{R}^n)$. The form q is called summably form bounded with respect to $-\Delta$ if, in addition, there are constants $a_j \ge 0$, $b_j \ge 0$ such that

$$\sum_{j \in \mathbb{Z}^n} (a_j + b_j) < \infty \tag{C.17}$$

and

$$|q(\phi, \phi)| \le a_j \|\nabla\phi\|^2 + b_j \|\phi\|^2, \qquad j \in J, \tag{C.18}$$

for all $\phi \in H^{2,1}(\mathbb{R}^n)$ with $\operatorname{supp}(\phi) \subset \bigcup_{|j-l|\le 1} \overline{C_l}$. Introducing the notation

$$f_{y_j}(x) = f(x + y_j), \quad q_{y_j}(f, g) = q(f_{y_j}, g_{y_j}), \qquad j \in J, \quad f, g \in H^{2,1}(\mathbb{R}^n), \tag{C.19}$$

we obtain

Lemma C.5. *Let q be summably form bounded with respect to $-\Delta$ on $H^{2,2}(\mathbb{R}^n)$ (with constants $a_j, b_j, j \in \mathbb{Z}^n$) and assume that q satisfies*

$$q(\chi f, g) = q(f, \bar{\chi} g) \tag{C.20}$$

for all $f, g \in H^{2,1}(\mathbb{R}^n)$ and all $\chi \in C_0^\infty(\mathbb{R}^n)$. Then

$$Q(f, g) = \sum_{j \in J} q_{y_j}(f, g), \qquad \mathscr{D}(Q) = H^{2,1}(\mathbb{R}^n) \tag{C.21}$$

is well defined and

$$|Q(f,f)| \le D\left(\sum_{j \in \mathbb{Z}^n} a_j\right) \|\nabla f\|^2 + \left[E \sum_{j \in \mathbb{Z}^n} a_j + \sum_{j \in \mathbb{Z}^n} b_j\right] \|f\|^2, \quad f \in H^{2,1}(\mathbb{R}^n), \tag{C.22}$$

where D and E are constants only depending on the set Y.

Next we specialize to one dimension and show that (III.2.1.6) and (III.3.5) define self-adjoint operators in $L^2(\mathbb{R})$. For this purpose we adopt the conventions chosen after (III.2.1.1) and define in $L^2(\mathbb{R})$

$$\ddot{H}_Y = -\frac{d^2}{dx^2}, \qquad \mathscr{D}(\ddot{H}_Y) = \{g \in H^{2,2}(\mathbb{R}) | g(y_j) = g'(y_j) = 0, j \in J\}. \tag{C.23}$$

Clearly, $\ddot{H}_Y$ as a closed restriction of $\dot{H}_Y$ in (III.2.1.2) and of $\dot{H}_Y'$ in (III.3.1) is nonnegative and has deficiency indices (∞, ∞). We have

Lemma C.6. *Let $J_0 \subset J$ and let $a_j, b_j, c_j, d_j, j \in J_0$, be complex numbers satisfying*

$$\begin{aligned} &a_j \bar{c}_j - \bar{b}_j d_j = 1, \\ &\operatorname{Im}(\bar{a}_j b_j) = \operatorname{Im}(\bar{a}_j c_j) = \operatorname{Im}(\bar{a}_j d_j) = \operatorname{Im}(\bar{b}_j c_j) = \operatorname{Im}(\bar{c}_j d_j) = 0, \quad j \in J_0. \end{aligned} \tag{C.24}$$

Moreover, let

$$\xi_1^j(x) = 1, \qquad \xi_2^j(x) = x - y_{j+1}, \qquad x \in (y_j, y_{j+1}), \quad j \in J. \tag{C.25}$$

Then the operator H_ξ in $L^2(\mathbb{R})$ defined by

$$H_\xi = -\frac{d^2}{dx^2},$$

$$\begin{aligned} \mathscr{D}(H_\xi) = \{g \in H^{2,2}(\mathbb{R} - Y)| \\ &\forall j \in J_0\colon W(g, \xi_1^j)_{y_j+} + a_j W(g, \xi_1^{j-1})_{y_j-} = b_j W(g, \xi_2^{j-1})_{y_j-}, \\ &\qquad W(g, \xi_2^j)_{y_j+} + c_j W(g, \xi_2^{j-1})_{y_j-} = d_j W(g, \xi_1^{j-1})_{y_j-}; \\ &\forall j \in J - J_0\colon \text{either } g(y_{j\pm}) = 0 \text{ or } g'(y_{j\pm}) = 0\} \end{aligned} \tag{C.26}$$

(*W being the Wronskian*) *is a self-adjoint extension of* $\dot{H}_Y$. (*In obvious notation the last boundary conditions in* (C.26) *should be omitted in case* $J_0 = J$.)

It remains to apply Lemma C.6 to $-\Delta_{\alpha,Y}$ and $\Xi_{\beta,Y}$. Without loss of generality we may assume $J_0 = J$ (implying $\alpha_j, \beta_j \in \mathbb{R}$ for all $j \in J$). In the case of $-\Delta_{\alpha,Y}$ we choose

$$a_j = -1, \qquad b_j = -\alpha_j, \qquad c_j = (y_j - y_{j+1})\alpha_j - 1, \qquad d_j = y_j - y_{j+1},$$
$$\alpha_j \in \mathbb{R}, \quad j \in J, \tag{C.27}$$

and for $\Xi_{\beta,Y}$ we choose

$$a_j = -1, \qquad b_j = 0, \qquad c_j = -1, \qquad d_j = (y_j - y_{j+1}) - \beta_j,$$
$$\beta_j \in \mathbb{R}, \quad j \in J. \tag{C.28}$$

Taking into account that

$$\begin{aligned} &W(g, \xi_1^j)_{y_j+} = -\overline{g'(y_{j+})}, \qquad W(g, \xi_1^{j-1})_{y_j-} = -\overline{g'(y_{j-})}, \\ &W(g, \xi_2^{j-1})_{y_j+} = \overline{g(y_{j+})} - \overline{g'(y_{j+})}(y_j - y_{j+1}), \\ &W(g, \xi_2^{j-1})_{y_j-} = \overline{g(y_{j-})}, \qquad j \in J, \end{aligned} \tag{C.29}$$

one immediately verifies that the boundary conditions in (C.26) are equivalent to those in (III.2.1.6) and (III.3.5).

Finally, we show that $-\Delta_{\alpha,Y}$ is the operator uniquely associated with the form in $L^2(\mathbb{R})$

$$\begin{aligned} &Q_{\alpha,Y}(f, g) = (f', g') + \sum_{j\in J} \alpha_j \overline{f(y_j)} g(y_j), \qquad \alpha_j \in \mathbb{R}, \\ &\mathscr{D}(Q_{\alpha,Y}) = H^{2,1}(\mathbb{R}). \end{aligned} \tag{C.30}$$

For this purpose we recall that

$$\mathscr{D}_0(-\Delta_{\alpha,Y}) = \{g \in \mathscr{D}(-\Delta_{\alpha,Y}) | \operatorname{supp}(g) \text{ compact}\} \tag{C.31}$$

is a core for $-\Delta_{\alpha,Y}$ (cf. the discussion following (III.2.1.10)). On the other hand, since by Lemma C.5 $C_0^\infty(\mathbb{R} - Y)$ is a core for $Q_{\alpha,Y}$, we infer that $\mathscr{D}_0(-\Delta_{\alpha,Y})$ is also a core for $Q_{\alpha,Y}$. But for $\phi, \psi \in \mathscr{D}_0(-\Delta_{\alpha,Y})$ the equality

$$Q_{\alpha,Y}(\phi, \psi) = (\phi, [-\Delta_{\alpha,Y}]\psi) \tag{C.32}$$

is easily shown by integration by parts. This proves the above claim concerning $-\Delta_{\alpha,Y}$ and $Q_{\alpha,Y}$.

Notes

Theorem C.1 appeared in [115] and is based on corresponding results of [67] for the Dirac operator (see also [278]). We also refer to [345] for the stability of operator- and form-bounds in connection with Schrödinger operators with separated singularities of the potential. For general stability results of the deficiency index, cf. [68]. The explicit determination of deficiency indices of singular Schrödinger operators is discussed in [69], [378], [470], [471], and [512]. In the special case of spherically symmetric interactions, see, e.g., [158], [353], and [389]. General self-adjoint extensions of elliptic operators with boundary conditions on a closed set of measure zero are treated in [299], [470], [471].

Lemma C.2 is due to J. Brasche (private communication).

The proof of (C.7) can be found in [251].

We are indebted to P. Deift for the counterexample following Lemma C.3.

Theorem C.4 is due to [251].

Lemma C.5 follows from Satz 4 in [286] which extends previous results of Morgan [345].

Lemma C.6 is a special case of a much more general result (including potentials strongly singular on a discrete subset of $\mathbb{R}$) proven in [208].

APPENDIX D

Boundary Conditions for Schrödinger Operators on $(0, \infty)$

In $L^2((0, \infty))$ we consider the minimal Schrödinger operator

$$\dot{h} = -\frac{d^2}{dr^2} + \lambda(\lambda - 1)r^{-2} + \gamma r^{-1} + \alpha r^{-a} + W, \qquad \mathscr{D}(\dot{h}) = C_0^\infty((0, \infty)),$$

$$W \in L^\infty((0, \infty)) \text{ real-valued}, \quad \alpha, \gamma \in \mathbb{R}, \quad 0 < a < 2, \quad \tfrac{1}{2} \leq \lambda < \tfrac{3}{2}. \tag{D.1}$$

Due to our conditions on λ, the closure of $\dot{h}$, denoted by h, has deficiency indices (1, 1). In order to determine all self-adjoint extensions of h we study solutions of the equation

$$-\psi''(r) + [\lambda(\lambda - 1)r^{-2} + V(r)]\psi(r) = 0, \qquad r > 0, \tag{D.2}$$

where

$$V(r) = \gamma r^{-1} + \alpha r^{-a} + W(r). \tag{D.3}$$

The regular solution $F_\lambda(r)$ associated with (D.2) satisfies

$$F_\lambda(r) = F_\lambda^{(0)}(r) - \int_0^r dr'\, g_\lambda^{(0)}(r, r')V(r')F_\lambda(r'), \tag{D.4}$$

where

$$F_\lambda^{(0)}(r) = r^\lambda, \qquad G_\lambda^{(0)}(r) = \begin{cases} -r^{1/2}\ln r, & \lambda = \frac{1}{2}, \\ (2\lambda - 1)^{-1} r^{1-\lambda}, & \frac{1}{2} < \lambda < \frac{3}{2}, \end{cases} \tag{D.5}$$

and

$$g_\lambda^{(0)}(r, r') = G_\lambda^{(0)}(r)F_\lambda^{(0)}(r') - G_\lambda^{(0)}(r')F_\lambda^{(0)}(r). \tag{D.6}$$

By iterating (D.4) one proves

$$c_1(r_0)r^\lambda \le |F_\lambda(r)| \le c_2(r_0)r^\lambda, \qquad \tfrac{1}{2} \le \lambda < \tfrac{3}{2}, \quad r \le r_0, \tag{D.7}$$

for appropriate constants $r_0 > 0$, $c_j(r_0) > 0$, $j = 1, 2$. The irregular solution $G_\lambda(r)$ corresponding to (D.2) is then given by

$$G_\lambda(r) = F_\lambda(r) \int_r^{r_0} dr'[F_\lambda(r')]^{-2}, \qquad \tfrac{1}{2} \le \lambda < \tfrac{3}{2}, \quad r \le r_0, \tag{D.8}$$

implying

$$|G_\lambda(r)| \le c_3(r_0)G_\lambda^{(0)}(r), \qquad \tfrac{1}{2} \le \lambda < \tfrac{3}{2}, \quad r \le r_0. \tag{D.9}$$

Iteration and explicit integration in (D.4) (using (D.3)) yields an asymptotic expansion for $F_\lambda(r)$ as $r \downarrow 0$ which in turn after insertion into (D.8) gives a corresponding asymptotic expansion of $G_\lambda(r)$ as $r \downarrow 0$. Let $G_\lambda^{\mathrm{B}}(r)$ denote the asymptotic expansion of $G_\lambda(r)$ up to the order r^t, $t \le 2\lambda - 1$. Then we have

Theorem D.1. *Assume conditions* (D.1). *Then all self-adjoint extensions h_ν of h can be characterized by*

$$h_\nu = -\frac{d^2}{dr^2} + \lambda(\lambda - 1)r^{-2} + \gamma r^{-1} + \alpha r^{-a} + W,$$

$$\begin{aligned}\mathscr{D}(h_\nu) = \{g \in L^2((0, \infty)) | g, g' \in AC_{\mathrm{loc}}((0, \infty));\ \nu g_{0,\lambda} = g_{1,\lambda};\\ -g'' + \lambda(\lambda - 1)r^{-2}g + \gamma r^{-1}g + \alpha r^{-a}g \in L^2((0, \infty))\},\\ -\infty < \nu \le \infty, \quad \tfrac{1}{2} \le \lambda < \tfrac{3}{2}, \quad \alpha, \gamma \in \mathbb{R}, \quad 0 < a < 2.\end{aligned} \tag{D.10}$$

Here the boundary values $g_{0,\lambda}$ and $g_{1,\lambda}$ are defined as

$$\begin{aligned} g_{0,\lambda} &= \lim_{r\downarrow 0} g(r)/G_\lambda^{(0)}(r),\\ g_{1,\lambda} &= \lim_{r\downarrow 0} [g(r) - g_{0,\lambda}G_\lambda^{B}(r)]/F_\lambda^{(0)}(r), \qquad g \in \mathscr{D}(h^*).\end{aligned} \tag{D.11}$$

The boundary condition $g_{0,\lambda} = 0$ (i.e., $\nu = \infty$) represents the Friedrichs extension of h.

We end up with two special cases in which the computation of $G_\lambda^{\mathrm{B}}(r)$ is particularly simple. These cases are sufficient for our purposes in the text (for the general case, cf. [115]):

(A) $\lambda = \frac{1}{2}$ (the s-wave Schrödinger operator in two dimensions, cf. Ch. I.5)

Then

$$G_{1/2}^{\mathrm{B}}(r) = G_{1/2}^{(0)}(r) = -r^{1/2} \ln r, \qquad r > 0. \tag{D.12}$$

(B) $\lambda = 1$, $a \in (0, \frac{3}{2}) - \{1\}$ (the s-wave Schrödinger operator in three dimensions, cf. Sect. I.2.1)

Then

$$G_1^{\mathrm{B}}(r) = 1 + \alpha[(2-a)(3-a)]^{-1}[1 + 2(1-a)^{-1}]r^{2-a} + \gamma r \ln r + (\gamma/2)r,$$

$$r > 0, \quad \alpha, \gamma \in \mathbb{R}, \quad a \in (0, \tfrac{3}{2}) - \{1\}. \quad \text{(D.13)}$$

In particular, if $\lambda = 1$ and $\alpha = \gamma = 0$ (cf. Sect. I.1.1) then the boundary values for $g \in \mathscr{D}(h^*)$ take on the familiar form

$$g_{0,1} = g(0+), \qquad g_{1,1} = g'(0+). \qquad \text{(D.14)}$$

Notes

The results in Appendix D are based on [115]. The special case $\alpha = 0$ has been treated earlier in [392], using different techniques.

APPENDIX E

Time-Dependent Scattering Theory for Point Interactions

By a simple trick we reduce the problem of existence and asymptotic completeness of wave operators and the connection between time-dependent and time-independent (stationary) scattering theory for point interactions to the corresponding problem of trace class (in fact, finite rank) perturbations of certain self-adjoint operators.

We rely on

Theorem E.1. *Let $A_l \geq 1$, $l = 1, 2$, be self-adjoint operators in a complex separable Hilbert space $\mathscr{H}$. Assume that*

$$A_1^{-n} - A_2^{-n} \in \mathscr{B}_1(\mathscr{H}) \tag{E.1}$$

for some $n \in \mathbb{N}$. Then the strong limits

$$\begin{aligned} \text{s-}\lim_{t \to \pm\infty} e^{itA_l} e^{-itA_m} P_{\text{ac}}(A_m) &= \text{s-}\lim_{t \to \mp\infty} e^{itA_l^{-1}} e^{-itA_m^{-1}} P_{\text{ac}}(A_m) \\ &= \text{s-}\lim_{t \to \mp\infty} e^{itA_l^{-n}} e^{-itA_m^{-n}} P_{\text{ac}}(A_m), \end{aligned}$$

$$l \neq m, \quad l, m = 1, 2, \tag{E.2}$$

exist and equal each other (invariance principle). Here $P_{\text{ac}}(A_l)$ denotes the projection onto the absolutely continuous subspace corresponding to A_l, $l = 1, 2$. In addition, the wave operators defined as

$$\Omega_{\pm}(A_l, A_m) = \text{s-}\lim_{t \to \pm\infty} e^{itA_l} e^{-itA_m} P_{\text{ac}}(A_m), \qquad l \neq m, \quad l, m = 1, 2, \tag{E.3}$$

are asymptotically complete, i.e.,

$$\operatorname{Ran} \Omega_+(A_l, A_m) = \operatorname{Ran} \Omega_-(A_l, A_m) = P_{\mathrm{ac}}(A_l)\mathscr{H}, \qquad l \neq m, \quad l, m = 1, 2. \tag{E.4}$$

Since $(-\Delta_{\alpha,Y} + E)^{-1} - (-\Delta + E)^{-1}$, for $E > 0$ large enough, is of rank N in the N-center case (in $n = 1, 2, 3$ dimensions), Theorem E.1 (with $m = 1$) immediately applies (analogously for $\Xi_{\beta,Y}$). Replacing $(-\Delta_{\alpha,Y}, -\Delta)$ by $((-\Delta_{\alpha,Y} + E)^{-1}, (-\Delta + E)^{-1})$, $E > 0$, sufficiently large, one can use the known eigenfunction expansions of $-\Delta_{\alpha,Y}$ (resp. $\Xi_{\beta,Y}$) together with Abelian limits to establish

$$\begin{aligned}(\Omega_\pm(-\Delta_{\alpha,Y}, -\Delta)g)(x) &= (\Omega_\mp((-\Delta_{\alpha,Y} + E)^{-1}, (-\Delta + E)^{-1})g)(x) \\ &= \operatorname*{s-lim}_{R\to\infty} (2\pi)^{-n/2} \int_{|k|\le R} k^{n-1}\, dk \int_{S^{(n-1)}} d\omega\, \Psi^{\pm}_{\alpha,Y}(k\omega, x)\hat{g}(k), \\ & \qquad\qquad n = 2, 3, \end{aligned} \tag{E.5}$$

where

$$\Psi^{-}_{\alpha,Y}(k\omega, x) = \Psi_{\alpha,Y}(k\omega, x), \qquad \Psi^{+}_{\alpha,Y}(k\omega, x) = \overline{\Psi_{\alpha,Y}(-k\omega, x)} \tag{E.6}$$

(cf. (II.1.5.1) and (II.4.32)). The fact that

$$\frac{d}{dt}\left[e^{it(-\Delta_{\alpha,Y}+E)^{-1}} e^{-it(-\Delta+E)^{-1}}\right] \tag{E.7}$$

is of finite rank considerably simplifies the analysis. The associated unitary scattering operator $\mathscr{S}(-\Delta_{\alpha,Y}, -\Delta)$ in $L^2(\mathbb{R}^n)$, $n = 2, 3$, is then given by

$$\mathscr{S}(-\Delta_{\alpha,Y}, -\Delta) = \Omega_+(-\Delta_{\alpha,Y}, -\Delta)^*\Omega_-(-\Delta_{\alpha,Y}, -\Delta), \qquad n = 2, 3. \tag{E.8}$$

Using (E.5), the invariance principle, and (E.7) one then shows by a standard procedure that $\mathscr{S}(-\Delta_{\alpha,Y}, -\Delta)$ is unitarily equivalent to the direct integral of the on-shell scattering operator $\mathscr{S}_{\alpha,Y}(k)$, $k > 0$ in $L^2(S^{(n-2)})$. Of course the analogous construction works for $-\Delta_{\alpha,Y}$ and $\Xi_{\beta,Y}$ in one dimension.

Notes

Theorem E.1 is due to Birman [90], for extensive discussions see [390], Ch. XI.3.

The standard way to derive (E.5) for three-dimensional potential scattering is described in [434], Ch. V.4 (cf. also [39], Ch. 10 and [390], Ch. X1.6). The corresponding connection between $\mathscr{S}(-\Delta_{\alpha,Y}, -\Delta)$ and $\mathscr{S}_{\alpha,Y}(k)$ using (E.5) is discussed in great detail in [434], Ch. V.5. Since in our case one can utilize (E.7), all arguments parallel the case where $-\Delta$ is perturbed by a finite rank interaction also called a separable potential (one only needs to exchange $-\Delta$ and $(-\Delta + E)^{-1}$, $E > 0$ large enough).

Eigenfunction expansions and scattering theory for general nonlocal interactions have been treated in [39], Ch. 8.3, [84], [270], and in [480], Chs. 3.4 and 3.6.

One-dimensional scattering theory is extensively discussed in [407].

APPENDIX F

Dirichlet Forms for Point Interactions

In this appendix we sketch how to obtain point interactions by the use of local Dirichlet forms in $n = 1, 2, 3$ dimensions.

Let $\phi \in L^2_{\text{loc}}(\mathbb{R}^n)$, $n \in \mathbb{N}$, be real-valued and define the minimal energy form $\dot{E}_\phi$ in $L^2(\mathbb{R}^n; \phi^2\, d^n x)$ by

$$\dot{E}_\phi(g, h) = \int_{\mathbb{R}^n} \phi^2(x)\, d^n x\, \overline{(\nabla g)(x)}(\nabla h)(x), \qquad \mathscr{D}(\dot{E}_\phi) = C_0^1(\mathbb{R}^n). \tag{F.1}$$

If $\dot{E}_\phi$ is closable, we denote its closure by E_ϕ and the unique self-adjoint, nonnegative operator in $L^2(\mathbb{R}^n, \phi^2\, d^n x)$ associated with E_ϕ by H_ϕ. Obviously, $H_\phi = \nabla^* \nabla$ where ∇ denotes the closure of $\nabla|_{C_0^1}(\mathbb{R}^n)$ in $L^2(\mathbb{R}^n; \phi^2\, d^n x)$. A sufficient condition for closability of $\dot{E}_\phi$ can be obtained as follows. Let $\Sigma \subset \mathbb{R}^n$ be a closed set of Lebesgue measure zero and assume in addition $\nabla\phi \in L^2_{\text{loc}}(\mathbb{R}^n - \Sigma)$ (∇ the distributional gradient in $C_0^\infty(\mathbb{R}^n - \Sigma)'$ the dual space of $C_0^\infty(\mathbb{R}^n - \Sigma)$). Then a careful investigation shows that $[-\nabla - 2\phi^{-1}(\nabla\phi)]|_{C_0^1(\mathbb{R}^n - \Sigma)}$ is a formal adjoint of $\nabla|_{C_0^1(\mathbb{R}^n)}$ in $L^2(\mathbb{R}^n; \phi^2\, d^n x)$. Since $C_0^1(\mathbb{R}^n - \Sigma)$ is dense in $L^2(\mathbb{R}^n; \phi^2\, d^n x)$, $\dot{E}_\phi$ is closable. More precisely, we have

Theorem F.1. *Let $\Sigma \subset \mathbb{R}^n$, $n \in \mathbb{N}$, be a closed set of Lebesgue measure zero, let $\phi \in L^2_{\text{loc}}(\mathbb{R}^n)$ be real-valued, and let $\nabla\phi \in L^2_{\text{loc}}(\mathbb{R}^n - \Sigma)$. Then $\dot{E}_\phi$ is closable in $L^2(\mathbb{R}^n; \phi^2\, d^n x)$ and*

$$H_\phi f = -\Delta f - 2\phi^{-1}(\nabla\phi)\nabla f, \qquad f \in C_0^2(\mathbb{R}^n - \Sigma). \tag{F.2}$$

If, in addition, $\phi^2 > 0$ almost everywhere with respect to $d^n x$ (i.e., if $\phi^2\, d^n x$ and $d^n x$ are equivalent) then the isometry $g \to \phi^{-1} g$ between $L^2(\mathbb{R}^n)$ and

$L^2(\mathbb{R}^n; \phi^2\, d^n x)$ takes H_ϕ into a self-adjoint, nonnegative operator H in $L^2(\mathbb{R}^n)$

$$H = \phi H_\phi \phi^{-1} = \phi \nabla^* \nabla \phi^{-1}. \tag{F.3}$$

In particular, if $\phi \in L^2(\mathbb{R}^n)$, then $H_\phi 1 = 0$ implies

$$H\phi = 0. \tag{F.4}$$

Next we apply this result to the one-center point interaction. Let

$$\phi_{\alpha,y}(x) = \begin{cases} e^{\alpha|x-y|/2}, & x, y \in \mathbb{R}, \quad \alpha \in \mathbb{R}, n = 1, \\ \begin{cases} H_0^{(1)}[2ie^{[-2\pi\alpha+\Psi(1)]}|x-y|], & x \in \mathbb{R}^2 - \{y\}, \quad \alpha \in \mathbb{R}, \\ 1, & \alpha = \infty, n = 2, \end{cases} \\ \begin{cases} e^{4\pi\alpha|x-y|}/|x-y|, & x \in \mathbb{R}^3 - \{y\}, \quad \alpha \in \mathbb{R}, \\ 1, & \alpha = \infty, n = 3. \end{cases} \end{cases} \tag{F.5}$$

Then $\phi_{\alpha,y} > 0$ and $\phi_{\alpha,y}$ fulfills the hypotheses of Theorem F.1 with

$$\Sigma = \begin{cases} \{y\} & \text{if } \alpha \neq 0 \text{ for } n = 1 \text{ resp. if } \alpha \in \mathbb{R} \text{ for } n = 2, 3, \\ \varnothing & \text{if } \alpha = 0 \text{ for } n = 1 \text{ resp. if } \alpha = \infty \text{ for } n = 2, 3. \end{cases} \tag{F.6}$$

Hence $\dot{E}_{\phi_{\alpha,y}}$ is closable. In the following we exclude the trivial case $\phi_{\alpha,y}(x) = 1$. Let $g \in C_0^1(\mathbb{R}^n)$ with $g(y) = 0$, $n = 1, 2, 3$, then $\phi_{\alpha,y}^{-1} g \in C_0^1(\mathbb{R}^n) \subset \mathscr{D}(\nabla)$ and a computation shows

$$E_{\phi_{\alpha,y}}(\phi_{\alpha,y}^{-1} g, \phi_{\alpha,y}^{-1} g) = \int_{\mathbb{R}^n} d^n x \left[|(\nabla g)(x)|^2 + \begin{Bmatrix} \alpha^2/4, & n = 1 \\ 4e^{2[-2\pi\alpha+\Psi(1)]}, & n = 2 \\ (4\pi\alpha)^2, & n = 3 \end{Bmatrix} |g(x)|^2 \right]. \tag{F.7}$$

For $g \in C_0^2(\mathbb{R}^n)$ with $g(y) = 0$ this implies $\phi_{\alpha,y}^{-1} g \in \mathscr{D}(H_{\phi_{\alpha,y}})$ and

$$(\phi_{\alpha,y} H_{\phi_{\alpha,y}} \phi_{\alpha,y}^{-1}) g = \left[-\Delta + \begin{Bmatrix} \alpha^2/4, & n = 1 \\ 4e^{2[-2\pi\alpha+\Psi(1)]}, & n = 2 \\ (4\pi\alpha)^2, & n = 3 \end{Bmatrix} \right] g. \tag{F.8}$$

As a consequence,

$$H_{\alpha,y} \equiv \phi_{\alpha,y} \left[H_{\phi_{\alpha,y}} - \begin{Bmatrix} \alpha^2/4, & n = 1 \\ 4e^{2[-2\pi\alpha+\Psi(1)]}, & n = 2 \\ (4\pi\alpha)^2, & n = 3 \end{Bmatrix} \right] \phi_{\alpha,y}^{-1}$$

is a self-adjoint extension of $-\Delta$ defined on $g \in C_0^2(\mathbb{R}^n)$ with $g(y) = 0$. For $\alpha < 0$ if $n = 1, 3$ and for all $\alpha \in \mathbb{R}$ if $n = 2$ we have $\phi_{\alpha,y} \in L^2(\mathbb{R}^n)$ and hence $\phi_{\alpha,y}$ is the ground state of $H_{\alpha,y}$, i.e., $H_{\alpha,y}\phi_{\alpha,y} = 0$. Thus $H_{\alpha,y} = -\Delta_{\alpha,y}$ in these cases. Actually, since $\phi_{\alpha,y}$ satisfies the boundary condition for elements in $\mathscr{D}(-\Delta_{\alpha,y})$ in a neighborhood of the point y we obtain $H_{\alpha,y} = -\Delta_{\alpha,y}$ for all $\alpha \in \mathbb{R}$, $n = 1$, 2, 3. In the case $\alpha \geq 0$ for $n = 1, 3$ (i.e., in the case where $\phi_{\alpha,y} \notin L^2(\mathbb{R}^n)$) $\phi_{\alpha,y}$ represents a resonance function of $-\Delta_{\alpha,y}$. If $\alpha > 0$, $n = 1, 3$, then $\phi_{\alpha,y}$ can as well be replaced by the corresponding zero-energy scattering wave function (cf., e.g., (I.1.4.11))

$$\Psi_{\alpha,y}(0,x) = \begin{cases} \alpha^{-1} + |x-y|/2, & n=1, \\ 1 + (4\pi\alpha|x-y|)^{-1}, & n=3; \quad 0 < \alpha \le \infty. \end{cases} \tag{F.9}$$

The N-center case is more involved as shown below. Let us first concentrate on the case $n = 3$ and without loss of generality assume that $|\alpha_j| < \infty$, $j = 1, \ldots, N$. Take $k = i\kappa$, $\kappa \in \mathbb{R}$, and consider $\Gamma_{\alpha,Y}(i\kappa)$. Since

$$\frac{\partial}{\partial\kappa}\Gamma_{\alpha,Y}(i\kappa) = (4\pi)^{-1}[e^{-\kappa|y_j - y_{j'}|}]_{j,j'=1}^{N} > 0, \qquad \kappa > 0, \tag{F.10}$$

is positive definite (this follows from $e^{-\kappa|y|} = c\int_{\mathbb{R}^3} d^3k\, \kappa(k^2+\kappa^2)^{-2}e^{iky}$, $c, \kappa > 0$, cf., e.g., [437], p. 35) all eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$ are strictly increasing with respect to $\kappa > 0$. Moreover, since the off-diagonal elements of $\Gamma_{\alpha,Y}(i\kappa)$, $\kappa \in \mathbb{R}$, are all negative, $\Gamma_{\alpha,Y}(i\kappa)$ generates a positivity preserving semigroup $e^{-t\Gamma_{\alpha,Y}(i\kappa)}$, $t \ge 0$, $\kappa \in \mathbb{R}$, in $\mathbb{C}^N$ ([391], p. 210). Consequently, the smallest eigenvalue of $\Gamma_{\alpha,Y}(i\kappa)$ is nondegenerate and we may choose a corresponding nonnegative eigenvector. Assume that there exists a $\kappa_0 \in \mathbb{R}$ such that $\Gamma_{\alpha,Y}(i\kappa_0)$ has zero as its smallest eigenvalue. Call $(c_1, \ldots, c_N)$, $c_j \ge 0$, $j = 1, \ldots, N$, the associated nonnegative eigenvector of $\Gamma_{\alpha,Y}(i\kappa_0)$. Then $\phi_{\alpha,Y}$ defined as

$$\phi_{\alpha,Y}(x) = \sum_{j=1}^{N} c_j e^{-\kappa_0|x-y_j|}/|x-y_j|, \qquad x \in \mathbb{R}^3 - Y, \tag{F.11}$$

fulfills all the assertions of Theorem F.1 with $\Sigma = Y$. (Actually we even have $c_j > 0, j = 1, \ldots, N$, since $c_{j_0} = 0$ for some j_0 would imply the vanishing of the point interaction at y_{j_0}, a fact which contradicts $|\alpha_{j_0}| < \infty$.) Consequently, the form $\dot{E}_{\phi_{\alpha,Y}}$ is closable and its closure gives rise to a uniquely associated operator $H_{\phi_{\alpha,Y}}$ in $L^2(\mathbb{R}^3;\, \phi_{\alpha,Y}^2\, d^3x)$. Again we have

$$\phi_{\alpha,Y}[H_{\phi_{\alpha,Y}} - \kappa_0^2]\phi_{\alpha,Y}^{-1} = -\Delta_{\alpha,Y}. \tag{F.12}$$

In case $\kappa_0 > 0$, $\phi_{\alpha,Y} \in L^2(\mathbb{R}^3)$ and hence it represents the ground state of $-\Delta_{\alpha,Y}$. If $\kappa_0 \le 0$ (i.e., if $\phi_{\alpha,Y} \notin L^2(\mathbb{R}^3)$), then $\phi_{\alpha,Y}$ is a resonance function of $-\Delta_{\alpha,Y}$. If no $\kappa_0 \ge 0$ exists, then $\phi_{\alpha,Y}$ can always be replaced by the zero-energy scattering wave function (cf. (II.1.5.1))

$$\Psi_{\alpha,Y}(0,x) = 1 + \sum_{j,j'=1}^{N} [\Gamma_{\alpha,Y}(0)]_{jj'}^{-1}(4\pi|x-y_j|)^{-1}, \qquad x \in \mathbb{R}^3 - Y. \tag{F.13}$$

Since by hypothesis all eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$, $\kappa \ge 0$, are strictly positive (i.e., $\inf\sigma(\Gamma_{\alpha,Y}(i\kappa)) > 0$, $\kappa \ge 0$), $[\Gamma_{\alpha,Y}(0)]^{-1}$ is positivity preserving implying $\Psi_{\alpha,Y}(0,x) \ge 1$.

For $n = 1, 2$ one can use similar arguments. Assume for simplicity that $\alpha_j \ne 0$ if $n = 1$ and $\alpha_j \in \mathbb{R}$ if $n = 2, j = 1, \ldots, N$. First of all, the eigenvalues of $\Gamma_{\alpha,Y}(i\kappa)$, $\kappa > 0$, are again strictly monotonously increasing for increasing $\kappa > 0$ since

$$-\frac{\partial}{\partial\kappa}G_{i\kappa}(y) = c\int_{\mathbb{R}^n} d^nk\, \kappa(k^2+\kappa^2)^{-2}e^{iky}, \quad c, \kappa > 0, \; y \in \mathbb{R}^n - \{0\}, \; n = 1, 2. \tag{F.14}$$

Second, $\Gamma_{\alpha,Y}(i\kappa)$, $\kappa > 0$, again generates a positivity preserving semigroup $e^{-t\Gamma_{\alpha,Y}(i\kappa)}$, $t \geq 0$, in $\mathbb{C}^N$ since all off-diagonal elements of $\Gamma_{\alpha,Y}(i\kappa)$, $\kappa > 0$, are negative. Hence one can construct a positive ground state (resp. a positive resonance function) of $-\Delta_{\alpha,Y}$ along the lines of (F.11) in case a suitable $\kappa_0 \in \mathbb{R}$ exists. One can also look for positive zero-energy scattering solutions. For example, if $n = 1$ the corresponding zero-energy solution (if it exists) reads

$$\Psi_{\alpha,Y}(0, x) = c\left\{1 + \sum_{j,j'=1}^{N} [\gamma_{\alpha,Y}]_{jj'}^{-1} |x - y_j|/2\right\}, \qquad c \in \mathbb{R}, \tag{F.15}$$

where

$$\gamma_{\alpha,Y} = [\alpha_j^{-1}\delta_{jj'} - |y_j - y_{j'}|/2]_{j,j'=1}^{N} \tag{F.16}$$

generates a positivity preserving semigroup $e^{-t\gamma_{\alpha,Y}}$, $t \geq 0$, in $\mathbb{C}^N$ (since its off-diagonal terms are negative). A careful check in the two-center case if $-\Delta_{\alpha,Y}$ has no bound states explicitly shows that $\Psi_{\alpha,Y}(0, x)$ can be chosen to be strictly positive if $[\gamma_{\alpha,Y}]^{-1}$ exists. A case distinction in the special case where $\det(\gamma_{\alpha,Y}) = 0$ shows that in this case too one can always find a strictly positive, locally absolutely continuous solution of $-\Delta_{\alpha,Y}\psi = 0$ which generates an appropriate local Dirichlet form for $-\Delta_{\alpha,Y}$.

If $n = 2$ no positive zero-energy scattering solution exists since $\ln|x - y_j|$ has no definite sign. In this case one always finds a strictly positive ground state of $-\Delta_{\alpha,Y}$ as discussed in Theorem II.4.2.

Notes

Theorem F.1 and the one-center treatment for $n = 3$ are taken from [32]. For further literature we refer, e.g., to [23], [25], [27], [33], [35], [192], [193], [396], [462], [495]. The possibility of constructing Dirichlet forms with zero-energy resonance (resp. zero-energy scattering wave functions) (cf. (F.9) and (F.13)) has been studied extensively in [23]. In the case of more general boundary conditions as discussed in [129], associated Dirichlet forms were constructed in [108].

APPENDIX G

Point Interactions and Scales of Hilbert Spaces

Let $H_m(\mathbb{R}^n)$, $n \in \mathbb{N}$, $m \in \mathbb{Z}$, denote the Sobolev spaces in momentum representation

$$H_m(\mathbb{R}^n) = L^2(\mathbb{R}^n; (p^2 + 1)^m \, d^n p), \qquad n \in \mathbb{N}, \quad m \in \mathbb{Z}, \tag{G.1}$$

yielding the scale of Hilbert spaces

$$\cdots \subset H_2(\mathbb{R}^n) \subset H_1(\mathbb{R}^n) \subset H_0(\mathbb{R}^n) \subset H_{-1}(\mathbb{R}^n) \subset H_{-2}(\mathbb{R}^n) \subset \cdots . \tag{G.2}$$

Since we are interested in "$\delta_n(\cdot - y)$-interactions" which correspond to plane waves in p-space

$$e_n^y(p) = (2\pi)^{-n/2} e^{-ipy}, \qquad p, y \in \mathbb{R}^n, \quad n \in \mathbb{N}, \tag{G.3}$$

we note

$$\begin{aligned}
&e_1^y \in H_{-1}(\mathbb{R}) \subset H_{-2}(\mathbb{R}), \\
&e_n^y \notin H_{-1}(\mathbb{R}^n), \qquad e_n^y \in H_{-2}(\mathbb{R}^n), \qquad n = 2, 3, \\
&e_n^y \notin H_{-2}(\mathbb{R}^n), \qquad n \geq 4.
\end{aligned} \tag{G.4}$$

In one dimension one can, in addition, study "$\delta'(\cdot - y)$-interactions" (i.e., "dipoles") since

$$d_1^y(p) = (2\pi)^{-1/2} p e^{-ipy}, \qquad p, y \in \mathbb{R}, \tag{G.5}$$

fulfills

$$d_1^y \notin H_{-1}(\mathbb{R}), \qquad d_1^y \in H_{-2}(\mathbb{R}). \tag{G.6}$$

We incidentally note that $e_n^y \notin H_{-2}(\mathbb{R}^n)$ for $n \geq 4$ is intimately connected with the fact that $-\Delta|_{C_0^\infty(\mathbb{R}^n - \{y\})}$ is essentially self-adjoint in $L^2(\mathbb{R}^n)$, $n \geq 4$, and hence ordinary point interactions are confined to dimensions 1, 2, and 3. Similarly, the exceptional case $e_1^y \in H_{-1}(\mathbb{R})$ is the reason that quadratic form methods are sufficient to discuss δ-interactions in one dimension. To simplify the notation we suppress the n-dependence in $H_m(\mathbb{R}^n)$ and simply write H_m from now on.

Let

$$R(E) = (p^2 - E)^{-1}, \qquad R(E)^{1/2} = (p^2 - E)^{-1/2}, \qquad E \in \mathbb{C} - [0, \infty), \quad \text{(G.7)}$$

with $R(E)^{1/2}$ the positive square root for $E < 0$. We note

Lemma G.1. *Let $E, E' < 0$. Then*

(i) *$R(E)$ satisfies the identities*

$$R(E) - R(E') = (E - E')R(E)R(E'), \qquad \frac{d}{dE}R(E) = R(E)^2. \quad \text{(G.8)}$$

(ii) *$R(E)$: $H_m \to H_{m+2}$, $m \in \mathbb{Z}$, is a topological isomorphism (i.e., a bounded onto map with bounded inverse).*

(iii) *$R(E)^{1/2}$: $H_m \to H_{m+1}$, $m \in \mathbb{Z}$, is a topological isomorphism.*

In the usual way the scalar product in H_0 can be extended to some pairs of vectors in H_{-2} making H_{-2} a partial inner product space: Let $\phi, \psi \in H_{-2}$ such that $\phi \in H_r$ and $\psi \in H_{-r}$ with $-2 \leq r \leq 2$. Then

$$\int_{\mathbb{R}^n} d^n p\, \overline{\phi(p)}\psi(p) = \int_{\mathbb{R}^n} d^n p\, (p^2 + 1)^{r/2}\overline{\phi(p)}(p^2 + 1)^{-r/2}\psi(p) \qquad \text{(G.9)}$$

is absolutely convergent and defines the partial inner product

$$\langle \phi | \psi \rangle = \int_{\mathbb{R}^n} d^n p\, \overline{\phi(p)}\psi(p). \qquad \text{(G.10)}$$

We observe that

$$\langle \phi | R(E)\psi \rangle \text{ exists for all } \phi, \psi \in H_{-1}, \qquad E \in \mathbb{C} - [0, \infty), \qquad \text{(G.11)}$$

while

$$\langle \phi' | R(E)^2\psi' \rangle \text{ exists for all } \phi', \psi' \in H_{-2}, \qquad E \in \mathbb{C} - [0, \infty). \quad \text{(G.12)}$$

Next we define the notation of a dyadic operator $|\psi'\rangle\langle\psi''|$, $\psi', \psi'' \in H_{-2}$ as follows: Let $H_{r'}$ (resp. $H_{r''}$) be the smallest space H_r that contains ψ' (resp. ψ''). Then $|\psi'\rangle\langle\psi''|$ denotes the bounded map

$$|\psi'\rangle\langle\psi''| \colon H_{-r''} \to H_{r'}, \qquad (|\psi'\rangle\langle\psi''|)(\phi) = \langle\psi''|\phi\rangle\psi'. \qquad \text{(G.13)}$$

Consequently, for any ψ', $\psi'' \in H_{-2}$ the symbol $R(E)|\psi'\rangle\langle\psi''|R(E)$ is a bounded operator in H_0 because its action on $g \in H_0$ by definition yields for $E \in \mathbb{C} - [0, \infty)$

$$(R(E)|\psi'\rangle\langle\psi''|R(E))(g) = \langle\chi''|R(E)g\rangle R(E)\psi' \in H_0, \qquad \text{(G.14)}$$

since $R(E)g \in H_2$ and $R(E)\psi' \in H_0$. Obviously, sums of dyadics and products with scalars can be defined in a straightforward way. The following shorthand notation turns out to be useful: Let

$$\Psi' = (\psi_1', \ldots, \psi_N') \in H_{-2}^N, \qquad \Psi'' = (\psi_1'', \ldots, \psi_N'') \in H_{-2}^N \tag{G.15}$$

(i.e., $\psi_j', \psi_j'' \in H_{-2}, j = 1, \ldots, N$) and $B = [B_{jj'}]_{j,j'=1}^N$ be any $N \times N$ matrix in $\mathbb{C}^N$. Then $|\Psi'\rangle B\langle\Psi''|$ is defined by

$$|\Psi'\rangle B\langle\Psi''| = \sum_{j,j'=1}^{N} |\psi_j'\rangle B_{jj'}\langle\psi_{j'}''| \tag{G.16}$$

and analogously $R(E)|\Psi'\rangle B\langle\Psi''|R(E)$ denotes the bounded operator in H_0

$$R(E)|\Psi'\rangle B\langle\Psi''|R(E) = \sum_{j,j'=1}^{N} R(E)|\psi_j'\rangle B_{jj'}\langle\psi_{j'}''|R(E), \qquad E \in \mathbb{C} - [0, \infty). \tag{G.17}$$

If $A_{s,r}$ denotes a bounded map from $H_r \subseteq H_0$ to $H_s \supseteq H_0$ its natural restriction A is defined as the restriction of $A_{s,r}$ to the domain

$$\mathscr{D}(A) = \{\phi \in H_r | A\phi \in H_0\} \subseteq H_0. \tag{G.18}$$

For instance, let

$$T_{r,r+2}: H_{r+2} \to H_r, \qquad (T_{r,r+2}\psi)(p) = p^2\psi(p), \qquad r \in \mathbb{Z}. \tag{G.19}$$

Then the natural restriction T of $T_{-1,1}$ (mapping H_1 into H_{-1}) equals the kinetic energy operator with $\mathscr{D}(T) = H_2$ its operator domain (i.e., $T = T_{0,2}$). In general, we note

Theorem G.2. *Let $\Phi = (\phi_1, \ldots, \phi_N) \in H_{-1}^N$ and $B = [B_{jj'}]_{j,j'=1}^N$ be an invertible matrix in $\mathbb{C}^N$. Then the natural restriction of $T_{-1,1} + |\Phi\rangle B\langle\Phi|$ (mapping H_1 into H_{-1}) denoted by S is a closed operator in H_0. The resolvent of S is given by*

$$(S - E)^{-1} = R(E) - R(E)|\Phi\rangle[\Omega(E)]^{-1}\langle\Phi|R(E),$$
$$E \in \mathbb{C} - [0, \infty), \quad \det[\Omega(E)] \neq 0, \tag{G.20}$$

where

$$\Omega(E)_{jj'} = \langle\phi_j|R(E)\phi_{j'}\rangle + B_{jj'}^{-1}, \qquad j, j' = 1, \ldots, N. \tag{G.21}$$

Moreover, S is self-adjoint in H_0 if B is Hermitian in $\mathbb{C}^N$.

In the case $\Psi \in H_{-2}^N$ but $\Psi \notin H_{-1}^N$ we get

Theorem G.3. *Let $\psi_j \in H_{-2}, \psi_j \notin H_{-1}, j = 1, \ldots, N$, be linearly independent over H_0 (i.e., no nontrivial linear combination $\sum_{j=1}^N \lambda_j\psi_j$ lies in H_0), $\Psi = (\psi_1, \ldots, \psi_N)$. If B is any invertible matrix in $\mathbb{C}^N$, the natural restriction of $T_{0,2} + |\Psi\rangle B\langle\Psi|$ (mapping H_2 into H_{-2}) is given by the restriction of $T_{0,2} \equiv T$ to the domain*

$$\{g \in H_2 | \langle\psi_j|g\rangle = 0, j = 1, \ldots, N\}. \tag{G.22}$$

Next let $\psi_j \in H_{-2}, j = 1, \dots, N$, be linearly independent over H_0 and define $\gamma_{jj'}(E)$ to be any solution of

$$\frac{d}{dE}\gamma(E)_{jj'} = -\langle\psi_j|R(E)^2\psi_{j'}\rangle, \qquad E \in \mathbb{C} - [0, \infty), \quad j, j' = 1, \dots, N. \quad \text{(G.23)}$$

Clearly, the most general solution of (G.23) is of the type

$$\gamma(E) + A, \quad \text{(G.24)}$$

where A is an arbitrary complex $N \times N$ matrix. In the special case where also $\psi_j \in H_{-1}, j = 1, \dots, N$, eq. (G.23) has the particular solution $-(\psi_j, R(E)\psi_{j'})$, $j, j' = 1, \dots, N$.

Theorem G.4. *Let $\psi_j \in H_{-2}, j = 1, \dots, N$, be linearly independent over H_0, $\Psi = (\psi_1, \dots, \psi_N)$ and let $\gamma(E)$, $E \in \mathbb{C} - [0, \infty)$, be a solution of* (G.23). *Define the bounded operator R_γ^Ψ in H_0 by*

$$R_\gamma^\Psi(E) = R(E) + R(E)|\Psi\rangle[\gamma(E)]^{-1}\langle\Psi|R(E),$$

$$E \in \mathbb{C} - [0, \infty), \quad \det[\gamma(E)] \neq 0. \quad \text{(G.25)}$$

Then $R_\gamma^\Psi(E)$ is the resolvent of a closed densely defined operator T_γ^Ψ in H_0

$$R_\gamma^\Psi(E) = (T_\gamma^\Psi - E)^{-1}, \qquad E \in \mathbb{C} - [0, \infty), \quad \det[\gamma(E)] \neq 0. \quad \text{(G.26)}$$

If $\gamma(E)$ is Hermitian for $E < 0$, then T_γ^Ψ is self-adjoint. Define $\gamma^*(E) = \gamma^{\mathrm{T}}(\bar{E})$, then $(T_\gamma^\Psi)^* = T_{\gamma^*}^\Psi$. Moreover, let $E_0 \in \mathbb{C} - [0, \infty)$, $\det[\gamma(E_0)] \neq 0$. Then the domain of T_γ^Ψ consists of all elements g of the type

$$g = g_{E_0} + R(E_0)|\Psi\rangle[\gamma(E_0)]^{-1}\langle\Psi|R(E_0), \quad \text{(G.27)}$$

where $g_{E_0} \in H_2$. The decomposition (G.27) *is unique and with $g \in \mathscr{D}(T_\gamma^\Psi)$ of this form we obtain*

$$(T_\gamma^\Psi - E_0)g = (T - E_0)g_{E_0}. \quad \text{(G.28)}$$

Finally, let

$$\mathscr{D}_0 = \{g \in H_2 | \langle\psi_j|g\rangle = 0, j = 1, \dots, N\}. \quad \text{(G.29)}$$

Then

$$\mathscr{D}(T_\gamma^\Psi) \cap H_2 = \mathscr{D}_0, \qquad T_\gamma^\Psi|_{\mathscr{D}_0} = T|_{\mathscr{D}_0}. \quad \text{(G.30)}$$

Next we discuss approximations for T_γ^Ψ. Let $\psi_j \in H_{-2}$, $j = 1, \dots, N$, be linearly independent over H_0 and assume that $\phi_j^\omega \in H_{-1}, \omega > 0, j = 1, \dots, N$, converge to ψ_j in H_{-2}-topology as $\omega \to \infty$, i.e., $\lim_{\omega\to\infty} \|\phi_j^\omega - \psi_j\|_{-2} = 0, j = 1, \dots, N$. A family M^ω of complex $N \times N$ matrices is called a *counterterm* for $\Psi^\omega = (\phi_1^\omega, \dots, \phi_N^\omega)$ iff

$$\lim_{\omega\to\infty} [\langle\phi_j^\omega|R(E)\phi_{j'}^\omega\rangle + M_{jj'}^\omega]_{j,j'=1}^N \quad \text{(G.31)}$$

exists for some (and hence for all) $E \in \mathbb{C} - [0, \infty)$.

Theorem G.5. *Let $\psi_j \in H_{-2}, j = 1, \ldots, N$, be linearly independent over H_0, $\Psi = (\psi_1, \ldots, \psi_N)$ and $\phi_j^\omega \in H_{-1}, \omega > 0, j = 1, \ldots, N$, with*

$$\lim_{\omega \to \infty} \|\phi_j^\omega - \psi_j\|_{-2} = 0, \qquad j = 1, \ldots, N. \tag{G.32}$$

Moreover, let the complex $N \times N$ matrix M^ω be a counterterm for $\Phi^\omega = (\phi_1^\omega, \ldots, \phi_N^\omega)$ such that M^ω is invertible for $\omega > 0$ large enough. Define

$$\gamma(E)_{jj'} = -\lim_{\omega \to \infty} [\langle \phi_j^\omega | R(E) \phi_{j'}^\omega \rangle + M_{jj'}^\omega], \qquad j, j' = 1, \ldots, N. \tag{G.33}$$

Then $\gamma(E)$ satisfies (G.23) *and hence defines an operator T_γ^Ψ and*

$$(T_\gamma^\Psi - E)^{-1} = \text{n-}\lim_{\omega \to \infty} (T \dot{+} |\Phi^\omega\rangle [M^\omega]^{-1} \langle \Phi^\omega| - E)^{-1}, \qquad E \in \mathbb{C} - \mathbb{R}, \tag{G.34}$$

where $\dot{+}$ denotes the form sum (i.e., the natural restriction of $T_{-1,1} + |\Phi^\omega\rangle [M^\omega]^{-1} \langle \Phi^\omega|$ mapping H_1 into H_{-1}).

Finally, we turn to concrete examples:

(a) δ-interactions in one dimension:

$$\begin{aligned} &\psi_j(p) = e_1^{y_j}(p), \qquad p, y_j \in \mathbb{R}, \\ &\gamma(E)_{jj'} = -(2\kappa)^{-1} e^{-\kappa|y_j - y_{j'}|} + A_{jj'}, \qquad j, j' = 1, \ldots, N. \end{aligned} \tag{G.35}$$

(b) δ'-interactions in one dimension:

$$\begin{aligned} &\psi_j(p) = d_1^{y_j}(p), \qquad p, y_j \in \mathbb{R}, \\ &\gamma(E)_{jj'} = (\kappa/2) e^{-\kappa|y_j - y_{j'}|} + A_{jj'}, \qquad j, j' = 1, \ldots, N. \end{aligned} \tag{G.36}$$

(c) δ-interactions in two dimensions:

$$\psi_j(p) = e_2^{y_j}(p), \qquad p, y_j \in \mathbb{R}^2,$$

$$\gamma(E)_{jj'} = \begin{cases} (2\pi)^{-1} \ln \kappa + A_{jj}, & j = j' \\ -(2\pi)^{-1} K_0(\kappa |y_j - y_{j'}|) + A_{jj'}, & j \neq j', \ j, j' = 1, \ldots, N, \end{cases} \tag{G.37}$$

($K_0(\cdot)$ the modified irregular Bessel function of order zero [1]).

(d) δ-interactions in three dimensions:

$$\psi_j(p) = e_3^{y_j}(p), \qquad p, y_j \in \mathbb{R}^3,$$

$$\gamma(E)_{jj'} = \begin{cases} (4\pi)^{-1} \kappa + A_{jj}, & j = j' \\ -(4\pi |y_j - y_{j'}|)^{-1} e^{-\kappa|y_j - y_{j'}|} + A_{jj'}, & j \neq j', \ j, j' = 1, \ldots, N, \end{cases} \tag{G.38}$$

where A is any complex $N \times N$ matrix and $E = -\kappa^2$, $\mathrm{Re}\,\kappa > 0$.

We note that in this context the condition $\langle \psi_j | g \rangle = 0$ in (G.29) simply means that the inverse Fourier transform of g vanishes at the points y_j, $j = 1, \ldots, N$.

If A is not a diagonal matrix, then different points y_j are connected by the boundary conditions. On the other hand, if A is diagonal the point interactions are independent (i.e., one has separated boundary conditions at each point y_j) and T_γ^Ψ coincides with $-\Delta_{\alpha,Y}$ by identifying

$$A_{jj'} = \begin{cases} -(1/\alpha_j)\delta_{jj'}, & n = 1, \\ [2\pi\alpha_j - \ln(2) - \Psi(1)]\delta_{jj'}, & n = 2, \\ \alpha_j\delta_{jj'}, & n = 3, \quad j, j' = 1, \ldots, N, \end{cases} \tag{G.39}$$

$$\gamma(E) = \Gamma(i\kappa), \qquad n = 1, 2, 3, \quad E = -\kappa^2, \quad \operatorname{Re}\kappa > 0. \tag{G.40}$$

Similarly, T_γ^Ψ coincides with $\Xi_{\beta,Y}$ identifying

$$A_{jj'} = (1/\beta_j)\delta_{jj'}, \qquad j, j' = 1, \ldots, N, \tag{G.41}$$

$$\gamma(E) = \kappa^2\Gamma(i\kappa), \qquad E = -\kappa^2, \quad \operatorname{Re}\kappa > 0. \tag{G.42}$$

In the three-dimensional case (G.38), approximations according to Theorem G.5 may be constructed as follows: Define the cut-off functions

$$\phi_j^\omega(p) = \chi_\omega(p)e_3^{y_j}(p),$$
$$\chi_\omega(p) = \begin{cases} 1, & |p| \le \omega, \\ 0, & |p| > \omega, \quad \omega > 0, \quad p, y_j \in \mathbb{R}^3, \quad j = 1, \ldots, N. \end{cases} \tag{G.43}$$

Then

$$M_{jj'}^\omega = -\left[\int_{\mathbb{R}^3} d^3p\,|p|^{-2}|\phi_j^\omega(p)|^2 + \alpha_j\right]\delta_{jj'} = -[(2\pi^2)^{-1}\omega + \alpha_j]\delta_{jj'},$$
$$\alpha_j \in \mathbb{R}, \quad j, j' = 1, \ldots, N, \tag{G.44}$$

represents a counterterm for $\Phi^\omega = (\phi_1^\omega, \ldots, \phi_N^\omega)$. Thus

$$T \dotplus \sum_{j=1}^N |\phi_j^\omega\rangle[-\alpha_j - (2\pi^2)^{-1}\omega]^{-1}\langle\phi_j^\omega| \tag{G.45}$$

converges to $H_\gamma^\Psi = -\Delta_{\alpha,Y}$ in norm resolvent sense as $\omega \to \infty$.

Locality of point interactions in the general case where the matrix A in (G.24) is not necessarily diagonal is described in

Theorem G.6. *Let $\psi_j(p) = e_n^{y_j}(p)$, $n = 1, 2, 3$, or $\psi_j(p) = d_1^{y_j}(p)$, $j = 1, \ldots, N$, $\Psi = (\psi_1, \ldots, \psi_N)$ and let $\gamma(E)$ be any solution of* (G.23). *Then T_γ^Ψ is local, i.e., if $g \in \mathscr{D}(T_\gamma^\Psi)$ vanishes in an open set $U \subseteq \mathbb{R}^n$, then $T_\gamma^\Psi g$ vanishes in U.*

The constructions in this appendix generalize to the infinite center case (the Kronig–Penney model and its two- and three-dimensional generalizations) [227]. We also emphasize that T can be replaced by any semibounded self-adjoint operator in H_0.

Notes

Appendix G is taken entirely from [226].

Partial inner product space are discussed, e.g., in [43], [44] and in [45].

APPENDIX H

Nonstandard Analysis and Point Interactions

H.1 A Very Short Introduction to Nonstandard Analysis

Nonstandard analysis is essentially analysis over a larger field of numbers than $\mathbb{R}$ (or $\mathbb{C}$), namely a field $^*\mathbb{R}$ (or $^*\mathbb{C}$) containing, in addition, infinitesimals and infinitely large numbers. We can construct a model for $^*\mathbb{R}$ as follows. Let m be a finitely additive measure on $\mathbb{N}$ such that

$$m(A) \in \{0, 1\}, \qquad A \subseteq \mathbb{N}, \tag{H.1}$$

and

$$|A| < \infty \Rightarrow m(A) = 0; \qquad m(\mathbb{N}) = 1. \tag{H.2}$$

The existence of measures of this type follows from, e.g., Zorn's lemma. In fact, the existence of m is equivalent to the so-called ultrafilter theorem which is weaker than Zorn's lemma. We denote sets $A \subseteq \mathbb{N}$ with $m(A) = 1$ as "big" and with $m(A) = 0$ as "small". Consider now sequences $a = \{a_n\}_{n \in \mathbb{N}}$, $b = \{b_n\}_{n \in \mathbb{N}}$, $a_n, b_n \in \mathbb{R}$, and define the equivalence relation $\sim$ as follows

$$a \sim b \quad \text{iff} \quad m(\{n \in \mathbb{N} \,|\, a_n = b_n\}) = 1 \tag{H.3}$$

and we write $a = b$ m-a.e. With these definitions we have

$$^*\mathbb{R} = \mathbb{R}^{\mathbb{N}}/\sim. \tag{H.4}$$

We call $^*\mathbb{R}$ the set of all hyperreals. For any sequence $a = \{a_n\}_{n \in \mathbb{N}}$ we let $\langle a \rangle$ denote its equivalence class with respect to $\sim$. One easily verifies

$$\langle a \rangle + \langle b \rangle = \langle a + b \rangle, \qquad \langle a \rangle \langle b \rangle = \langle ab \rangle \tag{H.5}$$

if we define addition and multiplication pointwise in $^*\mathbb{R}$. The zero for addition, denoted by 0, is the sequence with only zeros, while the unit of multiplication, denoted by 1, is the sequence with only ones. If $\langle a \rangle \neq 0$ we can define the its inverse $\langle a \rangle^{-1}$ by $(a^{-1})_n = (a_n)^{-1}$ whenever $a_n \neq 0$. The above definitions make $^*\mathbb{R}$ into a field of numbers. $^*\mathbb{R}$ can be linearly ordered by defining

$$\langle a \rangle < \langle b \rangle \quad \text{iff} \quad m(\{n \in \mathbb{N} | a_n < b_n\}) = 1. \tag{H.6}$$

We can consider $\mathbb{R}$ as embedded in $^*\mathbb{R}$ by identifying any $r \in \mathbb{R}$ with the sequence $^*r \in {}^*\mathbb{R}$ where all the elements equal r. This embedding is an order preserving homomorphism. From now on we will write r for the element $^*r \in {}^*\mathbb{R}$. It is easily seen that $\mathbb{R}$ is a proper subset of $^*\mathbb{R}$. For instance, we have

$$\langle \{n\}_{n \in \mathbb{N}} \rangle \in {}^*\mathbb{R} - \mathbb{R}, \qquad \left\langle \left\{\frac{1}{n}\right\}_{n \in \mathbb{N}} \right\rangle \in {}^*\mathbb{R} - \mathbb{R}, \tag{H.7}$$

with

$$\langle \{n\}_{n \in \mathbb{N}} \rangle \left\langle \left\{\frac{1}{n}\right\}_{n \in \mathbb{N}} \right\rangle = 1. \tag{H.8}$$

It is natural to call the number $\langle \{n\}_{n \in \mathbb{N}} \rangle$ "positive infinite" since it is strictly larger than any real number $r \in \mathbb{R}$, while it is natural to call the number $\langle \{1/n\}_{n \in \mathbb{N}} \rangle$ a "positive infinitesimal" since it is a positive number smaller than any positive real number $r \in \mathbb{R}$. More generally, we define $x \in {}^*\mathbb{R}$ as *infinitesimal* iff for all $r \in \mathbb{R}$

$$-r < x < r. \tag{H.9}$$

(Note that 0 is an infinitesimal by this definition.) Furthermore, $x \in {}^*\mathbb{R}$ is called *infinite* iff for all $r \in \mathbb{R}$

$$|x| > r, \tag{H.10}$$

where $|x| = \langle \{|a_n|\}_{n \in \mathbb{N}} \rangle$ for $x = \langle \{a_n\}_{n \in \mathbb{N}} \rangle$, and $x \in {}^*\mathbb{R}$ is called *finite* (or *near standard*) iff there exists an $r \in \mathbb{R}$ such that

$$|x| < r. \tag{H.11}$$

It is easily seen that any finite $x \in {}^*\mathbb{R}$ can be written uniquely as

$$x = r + \varepsilon \tag{H.12}$$

with $r \in \mathbb{R}$ and ε infinitesimal. r is then called the *standard part* of x and is denoted by

$$r = \mathrm{st}(x). \tag{H.13}$$

In fact, consider the set

$$S_x = \{s \in \mathbb{R} | s < x\}. \tag{H.14}$$

Then S_x is nonempty since $-s \in S_x$ with $s > |x|$ exists by assumption of x being finite. By Dedekind's completeness of $\mathbb{R}$, S_x has a supremum r in $\mathbb{R}$. We will show that $r = \mathrm{st}(x)$. In fact,

$$r - t \le x \le r + t, \qquad t \in (0, \infty). \tag{H.15}$$

From this we infer that $x - r$ is infinitesimal and thus $r = \mathrm{st}(x)$. To prove uniqueness we write

$$x = r_1 + \varepsilon_1 = r_2 + \varepsilon_2. \tag{H.16}$$

Then

$$\varepsilon_1 - \varepsilon_2 = r_1 - r_2 \tag{H.17}$$

is both infinitesimal and real, and hence it has to be equal to zero. We write

$$x \approx y \tag{H.18}$$

if $x - y$ is infinitesimal.

To do analysis on $^*\mathbb{R}$, one has to show how to extend (in a natural way) sets, functions, etc. from $\mathbb{R}$ to $^*\mathbb{R}$. The simplest objects with respect to this extension are called internal objects. We call any subset $A \subseteq {}^*\mathbb{R}$ *internal* iff there are sets $A_n \subseteq \mathbb{R}$, $n \in \mathbb{N}$, such that

$$A = \langle\{a_n\}_{n\in\mathbb{N}}\rangle \in {}^*\mathbb{R} | m(\{n \in \mathbb{N} | a_n \in A_n\}) = 1\}. \tag{H.19}$$

We write

$$A = \langle\{A_n\}_{n\in\mathbb{N}}\rangle. \tag{H.20}$$

Similarly, an internal function is a function F such that

$$F\colon {}^*\mathbb{R} \to {}^*\mathbb{R}, \qquad F(\langle\{a_n\}_{n\in\mathbb{N}}\rangle) = \langle\{F_n(a_n)\}_{n\in\mathbb{N}}\rangle, \quad \langle\{a_n\}_{n\in\mathbb{N}}\rangle \in {}^*\mathbb{R}, \tag{H.21}$$

for some sequence $\{F_n\}_{n\in\mathbb{N}}$ of functions on $\mathbb{R}$. We write

$$F = \langle\{F_n\}_{n\in\mathbb{N}}\rangle. \tag{H.22}$$

As examples of internal sets and functions we may take, e.g.,

$$[a, b] = \{x \in {}^*\mathbb{R} | a \le x \le b\}, \qquad a, b \in {}^*\mathbb{R}, \tag{H.23}$$

and

$$F(\{a_n\}_{n\in\mathbb{N}}) = \langle\{\sin(b_n a_n)\}_{n\in\mathbb{N}}\rangle \tag{H.24}$$

for any sequence $\{b_n\}_{n\in\mathbb{N}}$. However, e.g., the set of all infinite numbers and its characteristic function are not internal, and hence they are called *external* objects.

For internal objects one can roughly transfer the elementary properties which can be formulated within first-order logic (allowing quantifiers only on numbers, not on sets). This is a special case of the so-called *transfer principle*, see, e.g., [14]. In particular, internal sets form an algebra under Boolean operations. Special types of internal sets and functions are the so-called *standard* ones. A set $A \subseteq {}^*\mathbb{R}$ is called standard iff there exist sets $A_n \subseteq \mathbb{R}$, $n \in \mathbb{N}_0$, such that

$$A = \langle\{A_n\}_{n\in\mathbb{N}}\rangle; \qquad m(\{n \in \mathbb{N} | A_n = A_0\}) = 1. \tag{H.25}$$

We then write

$$A = {}^*A_0. \tag{H.26}$$

A function $F\colon {}^*\mathbb{R} \to {}^*\mathbb{R}$ is called standard if there exists functions $F_n\colon \mathbb{R} \to \mathbb{R}$, $n \in \mathbb{N}_0$, such that

$$F = \langle \{F_n\}_{n \in \mathbb{N}} \rangle, \qquad m(\{n \in \mathbb{N} \mid F_n = F_0\}) = 1 \tag{H.27}$$

and we write

$$F = {}^*F_0. \tag{H.28}$$

With these notions at hand we can do most of classical elementary analysis, e.g.,

(i) Limit of sequences.
Let $s = \{s_n\}$, and consider s as the function $s\colon \mathbb{N} \to \mathbb{R}$. Then it has a nonstandard extension ${}^*s\colon {}^*\mathbb{N} \to {}^*\mathbb{R}$, and the limit points of $\{s_n\}_{n \in \mathbb{N}}$ are exactly the points $\mathrm{st}({}^*s_\omega)$ for some infinite $\omega \in {}^*\mathbb{N}$. Hence $\lim_{n \to \infty} s_n = \sigma$ iff $\mathrm{st}({}^*s_\omega) = \sigma$ for all infinite $\omega \in {}^*\mathbb{N}$.

(ii) Continuity of functions.
Let $f\colon I \to \mathbb{R}$, $I \subseteq \mathbb{R}$. Then f is continuous at $x \in I$ iff ${}^*f(x) = {}^*f(y)$ for all $y \in {}^*I$, $y \approx x$. f is uniformly continuous on I iff ${}^*f(x) \approx {}^*f(y)$ for all $x, y \in {}^*I$.

(iii) Derivative of a function.
Let $f\colon I \to \mathbb{R}$, $I \subseteq \mathbb{R}$. Then $(df/dx)(x)$ exists at a point $x \in I$ iff

$$\frac{\Delta {}^*f(x)}{\Delta x} = \frac{{}^*f(x + \Delta x) - {}^*f(x)}{\Delta x} \tag{H.29}$$

is finite for all infinitesimals $\Delta x \neq 0$ and $\mathrm{st}(\Delta {}^*f(x)/\Delta x)$ is independent of Δx. In this case

$$\frac{df}{dx}(x) = \mathrm{st}\left(\frac{\Delta {}^*f(x)}{\Delta x}\right). \tag{H.30}$$

(iv) Riemann integral.
Let $f\colon [a, b] \to \mathbb{R}$ be a continuous function on $[a, b] \subseteq \mathbb{R}$. Then

$$\int_a^b dx\, f(x) = \mathrm{st}\left({}^*\sum_a^b {}^*f(x)\Delta x\right), \qquad \Delta x \approx 0, \quad \Delta x \neq 0. \tag{H.31}$$

However, to do more advanced analysis a more sophisticated construction is required. We define the so-called *superstructure* $V(\mathbb{R})$ over $\mathbb{R}$ recursively as follows. Let

$$V_0(\mathbb{R}) = \mathbb{R}, \qquad V_n(\mathbb{R}) = V_{n-1}(\mathbb{R}) \cup \mathscr{P}(V_{n-1}(\mathbb{R})), \qquad n \in \mathbb{N}, \tag{H.32}$$

where $\mathscr{P}(B)$ means the power set of a set B, i.e., the set of all subsets of B. Then

$$V(\mathbb{R}) = \bigcup_{n \in \mathbb{N}_0} V_n(\mathbb{R}). \tag{H.33}$$

Since ordered pairs (x, y), $x, y \in \mathbb{R}$, can be looked upon as $\{\{x\}, \{x, y\}\}$ and as such they are elements of $\mathscr{P}(\mathscr{P}(\mathbb{R}))$, we see that, e.g., the set of all functions on $\mathbb{R}$ is in $V(\mathbb{R})$. Let

$$W_n = \{f \in V(\mathbb{R})^{\mathbb{N}} | m(\{n \in \mathbb{N} | f(n) \in V_n(\mathbb{R})\}) = 1\} \tag{H.34}$$

and

$$W = \bigcup_{n \in \mathbb{N}} W_n. \tag{H.35}$$

We define an equivalence relation $\sim$ on W by

$$f \sim g \quad \text{iff} \quad m(\{n \in \mathbb{N} | f(n) = g(n)\}) = 1, \tag{H.36}$$

and as before we let $\langle f \rangle$ denote the equivalence class with representative f. Let

$$\Pi_{\sim} V(\mathbb{R}) = W/\sim. \tag{H.37}$$

We call $\Pi_{\sim} V(\mathbb{R})$ the *bounded ultrapower* associated with $V(\mathbb{R})$, and we have

$$\begin{aligned} &\langle f \rangle = \langle g \rangle \quad \text{iff} \quad f \sim g, \\ &\langle f \rangle \in \langle g \rangle \quad \text{iff} \quad m(\{n \in \mathbb{N} | f(n) \in g(n)\}) = 1. \end{aligned} \tag{H.38}$$

Observe that

$$\Pi_{\sim} V(\mathbb{R}) = \bigcup_{n=0}^{\infty} (W_n/\sim); \qquad {}^*\mathbb{R} = W_0/\sim. \tag{H.39}$$

One can embed $V(\mathbb{R})$ in $\Pi_{\sim} V(\mathbb{R})$ in a natural way. Namely, let $x \in V(\mathbb{R})$, hence $x \in V_n(\mathbb{R})$ for some $n \in \mathbb{N}_0$ and consider the sequence $\{x\}_{n \in \mathbb{N}}$ with all elements equal to x. Then $\{x\}_{n \in \mathbb{N}} \in W_n$, and we define

$$i\colon V(\mathbb{R}) \to \Pi_{\sim} V(\mathbb{R}), \qquad i(x) = \langle \{x\}_{n \in \mathbb{N}} \rangle. \tag{H.40}$$

The mapping i coincides with the $*$-mapping $*\colon \mathbb{R} \to {}^*\mathbb{R}$ previously defined on $V_0(\mathbb{R})$. Furthermore, we will now embed $\Pi_{\sim} V(\mathbb{R})$ into $V({}^*\mathbb{R})$ where $V({}^*\mathbb{R})$ is defined as $V(\mathbb{R})$ but with $\mathbb{R}$ replaced by ${}^*\mathbb{R}$. The mapping j is the identity on $W_0/\sim \; = {}^*\mathbb{R}$, and if j is defined on $W_n/\sim$, we define j on $(W_{n+1}/\sim \; - \; W_n/\sim)$ by

$$j(\langle f \rangle) = \{j(\langle g \rangle) | \langle g \rangle \in \langle f \rangle\}. \tag{H.41}$$

In this way we obtain a mapping

$$j\colon \Pi_{\sim} V(\mathbb{R}) \to V({}^*\mathbb{R}), \qquad j(W_n/\sim) \subseteq V_n({}^*\mathbb{R}). \tag{H.42}$$

Define now

$$*\colon V(\mathbb{R}) \to V({}^*\mathbb{R}), \qquad * \equiv j \circ i. \tag{H.43}$$

Then $*$ is an embedding of $V(\mathbb{R})$ in $V({}^*\mathbb{R})$ which coincides with the usual $*$-operation on numbers $r \in \mathbb{R}$, subsets $A \subset \mathbb{R}$, and functions $f\colon \mathbb{R} \to \mathbb{R}$. Observe that

$$*(V(\mathbb{R})) \equiv {}^*V(\mathbb{R}) \neq V({}^*\mathbb{R}). \tag{H.44}$$

We call elements in ${}^*V(\mathbb{R})$ *standard*, and elements of standard sets are called *internal*, i.e., B is internal iff there exists an $A \in V(\mathbb{R})$ such that $B \in {}^*A$. *External* elements are elements of $V({}^*\mathbb{R})$ which are not internal. For internal entities there is a natural "transfer of properties". Consider, e.g., the statement: Every upper bounded subset of $\mathbb{R}$ has a least upper bound. This statement transfers into: Every internal upper bounded subset of $^*\mathbb{R}$ has a least upper bound. This statement would be false without the restriction to internal subsets. Consider, e.g., the upper bounded subset of $^*\mathbb{R}$ consisting of all infinitesimals. This set has obviously no least upper bound in $^*\mathbb{R}$. Actually, one can prove that

$$A \subset \mathbb{R}, \qquad A \text{ internal iff } A \text{ finite.} \tag{H.45}$$

Moreover, one has "overflow" in the sense that if A is internal and contains all positive infinitesimals, then A also contains some real positive number. Furthermore, one also has "underflow" in the sense that if A is internal and $(0, \infty) \subseteq A$, then A contains some positive infinitesimals. One also has

$$A, B \text{ internal} \Rightarrow A \cap B, \qquad A \cup B, \qquad A \times B \text{ internal.} \tag{H.46}$$

This ends our brief account of the basic principles of nonstandard analysis. In the next section we will show how this can be used to give a natural realization of the Hamiltonian with point interactions.

H.2 Point Interactions Using Nonstandard Analysis

In this section we will show how to construct the self-adjoint Hamiltonian $-\Delta_{\alpha,0}$ with one point interaction located at the origin with strength α using nonstandard analysis.

Heuristically, we want to give a meaning to the operator

$$-\Delta + \lambda\delta, \tag{H.47}$$

δ being Dirac's delta function, and λ *infinitesimal.* It is natural to attempt a standard realization of this operator in the internal version of $L^2(\mathbb{R}^3)$, namely $^*L^2(\mathbb{R}^3)$, which is well defined as an element of $^*V(\mathbb{R})$. The Laplacian $-\Delta$ naturally extends by transfer to a self-adjoint operator in $^*L^2(\mathbb{R}^3)$ which for simplicity we also denote by $-\Delta$. The characteristic function

$$\chi_\varepsilon(x) = \begin{cases} 1, & |x| \le \varepsilon, \\ 0, & |x| > \varepsilon, \end{cases} \qquad \varepsilon \in (0, \infty), \tag{H.48}$$

also has a well-defined corresponding function, again denoted by χ_ε from $^*\mathbb{R}^3$ into $\{0, 1\}$ for any infinitesimal $\varepsilon \neq 0$. Define

$$\lambda = \lambda_\varepsilon(\alpha, \beta, \gamma) = -(\gamma + \tfrac{1}{2})^2 \left(\frac{\pi}{\varepsilon}\right)^2 + \frac{8\pi\alpha}{\varepsilon} + \beta, \qquad \alpha, \beta \in \mathbb{R}, \quad \gamma \in \mathbb{N}, \tag{H.49}$$

which is a certain infinite number in $^*\mathbb{R}$ when ε is infinitesimal. For any real $\varepsilon \neq 0$,

$$H_\lambda = -\Delta + \lambda\chi_\varepsilon \tag{H.50}$$

is a well-defined self-adjoint operator in $L^2(\mathbb{R}^3)$ bounded from below by $\min\{0, \lambda\}$. Hence by transfer there exists a well-defined self-adjoint extension, denoted by H_λ, in ${}^*L^2(\mathbb{R}^3)$ with the same lower bound (as embedded in ${}^*\mathbb{R}$) for any infinitesimal $\varepsilon > 0$.

Before we can state our main theorem we have to introduce some more definitions. A bounded operator T in ${}^*L^2(\mathbb{R}^3)$ is called near standard if for any $f \in {}^*L^2(\mathbb{R}^3)$, f near standard (i.e., there exists $g \in L^2(\mathbb{R}^3)$ such that $\|f - {}^*g\| \approx 0$) we have that Tf is near standard. A function $f\colon {}^*\mathbb{R}^3 \to {}^*\mathbb{R}^3$ is *S-continuous* at $a \in {}^*\mathbb{R}$ iff

$$\forall \varepsilon \in (0, \infty), \exists \delta \in (0, \infty), \qquad \forall x \in {}^*\mathbb{R}\colon |x - a| < \delta \Rightarrow |f(x) - f(a)| < \varepsilon. \quad \text{(H.51)}$$

We then have

Theorem H.1. *Let ε be a positive infinitesimal, and let $\lambda = \lambda_\varepsilon(\alpha, \beta, \gamma)$ be defined by* (H.49). *Then the operator*

$$H_\lambda = -\Delta + \lambda\chi_\varepsilon \quad \text{(H.52)}$$

is a self-adjoint operator in ${}^*L^2(\mathbb{R}^3)$ with lower bound 0 *if $\alpha \geq 0$ and $-(4\pi\alpha)^2$ if $\alpha < 0$. The resolvent $(H_\lambda - z)^{-1}$ is near standard if $z \in \mathbb{C} - \mathbb{R}$, and its integral kernel is S-continuous outside the diagonal. Furthermore,*

$$\operatorname{st}[(H_{\lambda_\varepsilon(\alpha,\beta,\gamma)} - k^2)^{-1}(x, x')] = (-\Delta_{\alpha,0} - k^2)^{-1}(x, x'),$$
$$k \in \mathbb{C} - \{4\pi\alpha i\}, \quad x \neq x', \quad x, x' \in \mathbb{R}^3, \quad \text{(H.53)}$$

independently of ε, β, and γ. If $a \in {}^*\mathbb{R}$ is finite, then

$$\operatorname{st}[(H_a - k^2)^{-1}(x, x')] = G_k(x - x'), \qquad \operatorname{Im} k > 0, \quad x \neq x', \quad x, x' \in \mathbb{R}^3. \quad \text{(H.54)}$$

If α equals a positive infinite number, then

$$\operatorname{st}[(H_{\lambda_\varepsilon(\alpha,\beta,\gamma)} - k^2)^{-1}(x, x')] = G_k(x - x'),$$
$$\operatorname{Im} k > 0, \quad x \neq x', \quad x, x' \in \mathbb{R}^3, \quad \text{(H.55)}$$

independently of ε, α, β and γ.

PROOF. We follow the decomposition of $L^2(\mathbb{R}^3)$ with respect to angular momenta used in the proof of Theorem I.1.1.1. Thus we can split $L^2(\mathbb{R}^3)$ in a rotationally symmetric part $\mathscr{H}_s$ and its orthogonal complement $\mathscr{H}_s^\perp$. Since the perturbation $\lambda\chi_\varepsilon$ is rotation invariant it suffices (cf. the proof of Theorem I.1.1.1) by transfer to study the restriction of $H_\lambda = -\Delta + \lambda\chi_\varepsilon$ to ${}^*\mathscr{H}_s$. By transfer of the unitary equivalence (I.1.1.8) it is enough to study

$$-\frac{d^2}{dr^2} + \lambda_\varepsilon(\alpha, \beta, \gamma)\chi_\varepsilon \quad \text{(H.56)}$$

in ${}^*L^2([0, \infty); dr)$ with a Dirichlet boundary condition at the origin. To this end, we first consider

$$h_a = -\frac{d^2}{dr^2} + a\chi_\varepsilon, \qquad a, \varepsilon \in \mathbb{R}, \quad \text{(H.57)}$$

in $L^2([0, \infty); dr)$ with both a and ε *real*. A short computation then shows

$$(h_a - k^2)^{-1}(x, x') = \begin{cases} (2ib_+k)^{-1}\phi_k(\varepsilon, a, x)\psi_k(\varepsilon, a, x'), & x \le x', \\ (2ib_+k)^{-1}\phi_k(\varepsilon, a, x')\psi_k(\varepsilon, a, x), & x \ge x', \\ \qquad \operatorname{Im} k > 0, \quad x \ne x', \quad x, x' \in [0, \infty), \end{cases} \tag{H.58}$$

where

$$\begin{aligned} \phi_k(\varepsilon, a, x) &= \begin{cases} \sin(\sqrt{k^2 - a}x), & 0 \le x \le \varepsilon, \\ b_+e^{kx} + b_-e^{-kx}, & x \ge \varepsilon, \end{cases} \\ \psi_k(\varepsilon, a, x) &= \begin{cases} c_+e^{i\sqrt{k^2-a}x} + c_-e^{-i\sqrt{k^2-a}x}, & 0 \le x \le \varepsilon, \\ e^{-ikx}, & x \ge \varepsilon, \end{cases} \end{aligned} \tag{H.59}$$

and

$$\begin{aligned} b_\pm &= \frac{1}{2}e^{\mp ik\varepsilon}\left[\sin\sqrt{k^2 - a\varepsilon}) \pm \frac{\sqrt{k^2 - a}}{k}\cos(\sqrt{k^2 - a}\varepsilon)\right], \\ c_\pm &= \frac{1}{2}\left(1 \mp \frac{k}{\sqrt{k^2 - a}}\right)e^{-i(k \pm \sqrt{k^2-a})\varepsilon}. \end{aligned} \tag{H.60}$$

By transfer this also holds for $x, x' \in {}^*[0, \infty)$, $x \ne x'$, $a \in {}^*\mathbb{R}$, and ε infinitesimal, $\varepsilon > 0$. Hence we infer that with the number a finite, $\operatorname{st}[(h_a - k^2)^{-1}(x, x')]$ equals the integral kernel of the resolvent of the Laplacian on $[0, \infty)$ with Dirichlet boundary conditions at the origin.

If a is infinite, we need $b_\pm$ finite and b_+ not infinitesimal to make $(h_a - k^2)^{-1}(x, x')$ near standard. From (H.58) we see that this requires $\sin(\sqrt{k^2 - a}\varepsilon)$ and $\sqrt{k^2 - a}\cos(\sqrt{k^2 - a}\varepsilon)$ to be finite. But then $\cos(\sqrt{k^2 - a}\varepsilon)$ has to be infinitesimal, which yields

$$\sqrt{k^2 - a}\varepsilon = (\gamma + \tfrac{1}{2})\pi + \eta, \qquad \gamma \in {}^*\mathbb{N}, \tag{H.61}$$

with η infinitesimal such that

$$\tilde{\alpha} = \frac{(-1)^\gamma}{4\pi}\sqrt{k^2 - a}\cos(\sqrt{k^2 - a}\varepsilon) \tag{H.62}$$

is near standard. Using (H.61) we see that $\tilde{\alpha}$ is near standard iff $\sqrt{k^2 - a}\sin\eta$ is near standard which again is equivalent to $\eta\varepsilon^{-1}$ being near standard. From (H.61) we have

$$a = -(\gamma + \tfrac{1}{2})^2\left(\frac{\pi}{\varepsilon}\right)^2 - 2\frac{\pi}{\varepsilon}(\gamma + \tfrac{1}{2})\frac{\eta}{\varepsilon} + k^2 - \left(\frac{\eta}{\varepsilon}\right)^2. \tag{H.63}$$

Introducing

$$\xi = \eta\varepsilon^{-1}, \qquad \xi_0 = \operatorname{st}(\eta\varepsilon^{-1}) \tag{H.64}$$

we get

$$\begin{aligned} \alpha = \operatorname{st}(\tilde{\alpha}) &= \frac{1}{4\pi}\operatorname{st}\left\{\frac{(\gamma + \frac{1}{2})\pi + \eta}{\varepsilon}(-1)^\gamma\cos[(\gamma + \tfrac{1}{2})\pi + \eta]\right\} \\ &= \frac{-1}{4\pi}\operatorname{st}\left[(\gamma + \tfrac{1}{2})\frac{\pi}{\varepsilon}\sin\eta + \xi\sin\eta\right] \\ &= -\frac{1}{4\pi}(\gamma + \tfrac{1}{2})\xi_0\pi, \qquad \gamma \in \mathbb{N}. \end{aligned} \tag{H.65}$$

Taking $\xi \in \mathbb{R}$, we find

$$a = -(\gamma + \tfrac{1}{2})^2 \left(\frac{\pi}{\varepsilon}\right)^2 + 8\pi\alpha\left(\frac{\pi}{\varepsilon}\right) + k^2 - \xi^2. \tag{H.66}$$

With this choice we obtain

$$\operatorname{st}(b_\pm) = \frac{(-1)^\gamma}{2}\left(1 \pm \frac{4\pi\alpha}{k}\right), \qquad \operatorname{st}(c_\pm) = \tfrac{1}{2}e^{\mp(\gamma+1/2)\pi}, \tag{H.67}$$

and hence $\operatorname{st}[(b_+ + b_-)/k(b_+ - b_-)] = 1/4\pi\alpha$. However, this implies that

$$\operatorname{st}\left[\frac{\phi_k(\varepsilon, a, \varepsilon)}{\phi_k'(\varepsilon, a, \varepsilon)}\right] = \frac{1}{4\pi\alpha}. \tag{H.68}$$

Writing

$$\Phi_k(\alpha, x) = \operatorname{st}[\phi_k(\varepsilon, a, x)], \qquad \Psi_k(\alpha, x) = \operatorname{st}[\psi_k(\varepsilon, a, x)] \tag{H.69}$$

we see that they satisfy

$$-\Phi_k'' - k^2\Phi_k = 0, \qquad -\Psi_k'' - k^2\Psi_k = 0 \tag{H.70}$$

with boundary conditions

$$4\pi\alpha\Phi_k(\alpha, 0) = \Phi_k'(\alpha, 0), \qquad \Psi_k(\alpha, x) \xrightarrow[x\to\infty]{} 0. \tag{H.71}$$

This proves that

$$\operatorname{st}[(h_a - k^2)^{-1}(x, x')] = (h_{0,\alpha} - k^2)^{-1}(x, x'), \quad \operatorname{Im} k > 0, \quad x \neq x', \quad x, x' \in [0, \infty), \tag{H.72}$$

where $h_{0,\alpha}$ is defined by (I.1.1.12). ∎

Observe that H_λ in the above theorem is given directly as a *-bounded perturbation of $-\Delta$ in $^*L^2(\mathbb{R}^3)$, and that $-\Delta_{\alpha,0}$ is obtained by taking standard parts.

Noticing that we can obtain $\delta(x)$ using nonstandard analysis as

$$\delta_\varepsilon(x) = \left(\frac{4\pi}{3}\varepsilon^3\right)^{-1} \chi_\varepsilon(x) \tag{H.73}$$

(if $\varepsilon > 0$ is real, δ_ε is a δ-sequence as $\varepsilon \to 0$) we can rewrite H_λ as

$$H_\lambda = -\Delta + \tilde{\lambda}_\varepsilon(\alpha, \beta, \gamma)\delta_\varepsilon, \tag{H.74}$$

where

$$\tilde{\lambda}_\varepsilon(\alpha, \beta, \gamma) = \frac{4\pi}{3}[-(\gamma + \tfrac{1}{2})^2\pi^2\varepsilon + 8\pi^2\alpha\varepsilon^2 + \beta\varepsilon^3]. \tag{H.75}$$

As our final result in this appendix we will show how to use nonstandard analysis to construct $-\Delta_{\alpha,Y}$ with $Y \subset \mathbb{R}^3$, $|Y| < \infty$, using the approach advocated in Sect. II.1.1.

Theorem H.2. *Let $\hat{H}^\omega$ be the self-adjoint operator defined by* (II.1.1.15). *Then*

$$\operatorname{st}[(\hat{H}^\omega - k^2)^{-1}(x, x')] = (-\hat{\Delta}_{\alpha,Y} - k^2)^{-1}(x, x'),$$
$$\operatorname{Im} k > 0, \quad x \neq x', \quad x, x' \in \mathbb{R}^3 - Y, \tag{H.76}$$

provided ω is positive infinite and

$$\mu_j(\omega)^{-1} = \frac{\omega}{2\pi^2} + \alpha_j, \qquad \alpha_j \in \mathbb{R}, \quad j = 1, \ldots, N. \tag{H.77}$$

PROOF. Let ω be positive infinite. By transfer $\hat{H}^\omega$ is well defined in ${}^*L^2(\mathbb{R}^3)$ with resolvent given by (II.1.1.16). We have

$$\mathrm{st}[(\phi^\omega_{y_j}, (p^2 - k^2)^{-1}\phi^\omega_{y_{j'}})] = G_k(y_j - y_{j'}), \qquad j \neq j', \quad j, j' = 1, \ldots, N. \tag{H.78}$$

With $\mu_j(\omega)$ defined by (H.77) we get

$$\mathrm{st}[\mu_j(\omega)^{-1} - (\phi^\omega_{y_j}, (p^2 - k^2)^{-1}\phi^\omega_{y_j})] = \alpha_j - \frac{ik}{4\pi}, \qquad j = 1, \ldots, N, \tag{H.79}$$

which proves (H.76). ∎

Notes

Nonstandard analysis can be looked upon as a mathematical realization of century-old attempts at using infinitesimal and infinite numbers in mathematics, without running into contradictions. It was introduced by Robinson at the end of the 1950s (important tools for Robinson's theory had been developed earlier in mathematical logic, in particular, in work by Skolem). Robinson's book [394] was very influential. A major development took place in the mid-1970s, through Loeb's decisive introduction of a suitable nonstandard tool for measure theory and probability theory. As a consequence the theory of stochastic processes has become one of the main domains of applications of nonstandard analysis. The study of differential equations and dynamical systems by techniques of nonstandard analysis was greatly influenced by the work of Nelson [355]. The results reported in this appendix are based on [12] and the book [14] to which we refer for additional references.

APPENDIX I

Elements of Probability Theory

We shall collect here some basic notions of probability theory needed in Ch. III.5.

A *probability space* $(\Omega, \mathscr{A}, P)$ consists of a set Ω, a σ-algebra $\mathscr{A}$ of subsets of Ω, and a σ-additive probability measure P (i.e., a positive measure with total mass one). The sets A in $\mathscr{A}$ are called measurable sets or *events*. $P(A)$ is the measure or probability of the event A. A statement which holds for all points ω in the complement of a set with P-measure zero is said to hold P-almost surely (P-a.s.) or P-almost everywhere (P-a.e.).

A *random* (or *stochastic*) *variable* X on $(\Omega, \mathscr{A}, P)$ with values in a measurable space $(S, \mathscr{B}(S))$, with S some set and $\mathscr{B}(S)$ a σ-algebra of subsets of S, is a measurable mapping from Ω into S. In the case where S equals $\mathbb{R}$ and $\mathscr{B}(S)$ is the Borel σ-algebra one speaks of a real-valued random variable, sometimes the same is also said when S equals $\bar{\mathbb{R}} = \mathbb{R} \cup \{\pm\infty\}$. P is called the underlying probability measure for X. The image P_X of P under X, defined by

$$P_X(B) = P(X^{-1}(B)), \qquad B \in \mathscr{B}(S), \tag{I.1}$$

is called the *distribution* (or *measure*, or *law*) *of* X (under P). One writes $P(X \in B)$ for $P(\{\omega \in \Omega | X(\omega) \in B\})$. Thus

$$P(X \in B) = P_X(B) = P(A) \tag{I.2}$$

with $A = X^{-1}(B)$.

Remark. If $S = \mathbb{R}$ one can also define the function $F_X(x) = P_X((-\infty, x))$ as the distribution function of the random variable X. $F_X(x)$ is thus the

P-probability of the event $\{\omega \in \Omega | X(\omega) < x\}$. The mapping $x \to F_X(x)$ satisfying $F_X(-\infty) = 0$, $F_X(+\infty) = 1$, is monotone increasing and left continuous. Vice versa any function with these properties uniquely determines a probability measure on $(\mathbb{R}, \mathscr{B}(\mathbb{R}))$, where $\mathscr{B}(\mathbb{R})$ is the σ-algebra of Borel subsets of $\mathbb{R}$.

For any family $\mathscr{E} \subset \mathscr{A}$ of events let $\sigma(\mathscr{E})$ denote the smallest σ-algebra containing $\mathscr{E}$. If X is a random variable one calls $\sigma(X)$ the *σ-algebra generated by X* which is by definition the smallest σ-algebra containing all preimages of sets in $\mathscr{B}(S)$ under X, thus $\sigma(X) = \sigma\{X^{-1}(B) | B \in \mathscr{B}(S)\}$.

A family $\{A_\alpha\}_{\alpha \in I}$, I an index set, of events (in a probability space $(\Omega, \mathscr{A}, P)$) is called *independent* if for any choice of finitely many indices $\alpha_1, \ldots, \alpha_n$ one has

$$P(A_{\alpha_1} \cap \cdots \cap A_{\alpha_n}) = \prod_{k=1}^{n} P(A_{\alpha_k}). \tag{I.3}$$

A family $\{\mathscr{A}_\alpha\}_{\alpha \in I}$ of σ-algebras is *independent* if every family $\{A_\alpha\}_{\alpha \in I}$, $A_\alpha \in \mathscr{A}_\alpha$, of events is independent.

A family $\{X_\alpha\}_{\alpha \in I}$ of random variables is called *independent* if the family of σ-algebras $\{\sigma(X_\alpha)\}_{\alpha \in I}$ is independent.

A *stochastic process* with index set K, state space $(S, \mathscr{B}(S))$, and underlying probability space $(\Omega, \mathscr{A}, P)$ is a family of random variables X_κ on $(\Omega, \mathscr{A}, P)$ indexed by K. Thus, for each $\kappa \in K$, X_κ is a $(\Omega, \mathscr{A}, P)$-random variable with values in $(S, \mathscr{B}(S))$.

If S is nice enough, e.g., a polish space (i.e., a complete, separable metric space) we have the following: Given an independent family of random variables $\{X_\alpha\}_{\alpha \in I}$ with values in S, it is possible to find a "coordinate" ("canonical") stochastic process $\{\hat{X}_\alpha\}_{\alpha \in I}$ on the probability space $(S^I, \mathscr{B}(S^I), \hat{P})$ such that

$$\begin{aligned} \hat{P}(\hat{X}_{\alpha_1} \in B_1, \ldots, \hat{X}_{\alpha_n} \in B_n) &= P(X_{\alpha_1} \in B_1, \ldots, X_{\alpha_n} \in B_n) \\ &= \prod_{k=1}^{n} P(X_{\alpha_k} \in B_k), \qquad B_k \in \mathscr{B}(S). \end{aligned} \tag{I.4}$$

Here $\mathscr{B}(S^I)$ is the σ-algebra generated by the cylinder subsets of S^I, i.e., by all subsets of the form $\{\hat{\omega} \in S^I | (\hat{\omega}(\alpha_1), \ldots, \hat{\omega}(\alpha_n)) \in B_1 \times \cdots \times B_n\}$, with $B_k \in \mathscr{B}(S)$, $\alpha_k \in I$, $k = 1, \ldots, n$. $(S^I, \mathscr{B}(S^I), \hat{P})$ can be looked upon as the product space $\prod_{\alpha \in I} (S_\alpha, \mathscr{B}(S_\alpha), P_\alpha)$, where $(S_\alpha, \mathscr{B}(S_\alpha))$ is a copy of $(S, \mathscr{B}(S))$ and $P_\alpha = P_{X_\alpha}$. The process $(\hat{X}, S^I, \mathscr{B}(S^I), \hat{P})$ can be viewed as a "realization" of the family $\{X_\alpha\}_{\alpha \in I}$ inasmuch as $\hat{X}_\alpha$ has the same distribution as X_α, since $\hat{P}_{X_\alpha}(B) = P_{X_\alpha}(B)$, $\alpha \in I$, $B \in \mathscr{B}(S)$. This is a simple case of a more general theorem by Kolmogorov, see, e.g., [59].

The random variables X_α in a family $\{X_\alpha\}_{\alpha \in I}$ are called *identically distributed* if their laws are identical, i.e., if P_{X_α} is independent of α. In the above case then, if X_α are independent and identically distributed, we have that P_α is independent of α.

Let $\{\mathscr{A}_n\}_{n \in \mathbb{N}}$ be a sequence of σ-algebras of events. The *tail σ-algebra* (σ-algebra of *tail events*) is by definition the σ-algebra $\mathscr{A}_\infty$ defined by

$$\mathscr{A}_\infty = \bigcap_{n \in \mathbb{N}} \sigma\left(\bigcup_{m=n}^{\infty} \mathscr{A}_m\right). \tag{I.5}$$

If $\mathscr{A}_n$ is generated by X_n, then

$$\mathscr{A}_\infty = \bigcap_{n \in \mathbb{N}} \sigma(\{X_m | m \geq n\}). \tag{I.6}$$

A well-known theorem by Kolmogorov (*Kolmogorov's* 0–1 *law*) says that if the $\mathscr{A}_n$ are independent then $\mathscr{A}_\infty$ is P-trivial in the sense that $P(A) = 0$ or $P(A) = 1$ for any $A \in \mathscr{A}_\infty$. In particular, if $\{X_n\}_{n \in \mathbb{N}}$ is a sequence of independent random variables the corresponding tail events have probability either 0 or 1.

Applying this to $X_n = \chi_{A_n}$, A_n independent events, $n \in \mathbb{N}$, we then get $P(\limsup_{n \in \mathbb{N}} A_n) \in \{0, 1\}$. In fact, by the Borel–Cantelli lemma, $P(\limsup_{n \in \mathbb{N}} A_n) = 0$ holds iff $\sum_{n \in \mathbb{N}} P(A_n) < \infty$, $P(\limsup_{n \in \mathbb{N}} A_n) = 1$ iff $\sum_{n \in \mathbb{N}} P(A_n) = \infty$ (actually for $\sum_{n \in \mathbb{N}} P(A_n) < \infty \Rightarrow P(\limsup_{n \in \mathbb{N}} A_n) = 0$ one does not need the independence assumption).

A *random field* X with index a subset K of $\mathbb{R}^m$ is a family of random variables X_κ, $\kappa \in K$. If K is invariant under some subgroup of $\mathbb{R}^m$ and

$$P(X_{\kappa_1 + \kappa} \in A_1, \ldots, X_{\kappa_n + \kappa} \in A_n) = P(X_{\kappa_1} \in A_1, \ldots, X_{\kappa_n} \in A_n),$$
$$\kappa_j \in K, \quad A_j \in \mathscr{A}, \quad j = 1, \ldots, n, \tag{I.7}$$

then $\{X_\kappa\}_{\kappa \in K}$ is called *K-homogeneous* (or *K-stationary*).

A measurable transformation T of a probability space $(\Omega, \mathscr{A}, P)$ in itself is called *ergodic* if for any A such that $T^{-1}(A) = A$ we have $P(A) = 0$ or $P(A) = 1$.

Notes

General references for probability theory are, e.g., [59], [109], [383]. A classical treatise on stochastic processes is [157]. For discussions of ergodic transformations see, e.g., [306], [312].

APPENDIX J

Relativistic Point Interactions in One Dimension

Following the strategy in Chs. III.2 and III.3 we briefly sketch how to analyze one-dimensional Dirac operators with point interactions by means of appropriate difference equations.

Let D_0 denote the free Dirac operator in the Hilbert space $L^2(\mathbb{R}) \otimes \mathbb{C}^2$

$$D_0 = D, \qquad D = -ic\frac{d}{dx} \otimes \sigma_1 + \tfrac{1}{2}c^2 \otimes \sigma_3 = \begin{bmatrix} \dfrac{c^2}{2} & -ic\dfrac{d}{dx} \\ -ic\dfrac{d}{dx} & -\dfrac{c^2}{2} \end{bmatrix}, \tag{J.1}$$

$\mathscr{D}(D_0) = H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2$,

where

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{J.2}$$

are Pauli matrices in $\mathbb{C}^2$ and $c > 0$ denotes the velocity of light. The corresponding free resolvent is then given by

$$R_k = (D_0 - z)^{-1}, \qquad z \in \mathbb{C} - \{(-\infty, -c^2/2] \cup [c^2/2, \infty)\} \tag{J.3}$$

with integral kernel

$$R_k(x - x') = (i/2c)\begin{bmatrix} \zeta & \operatorname{sgn}(x - x') \\ \operatorname{sgn}(x - x') & \zeta^{-1} \end{bmatrix} e^{ik|x-x'|},$$

$$\zeta(z) = [z + (c^2/2)]/ck(z), \qquad ck(z) = [z^2 - (c^4/4)]^{1/2},$$

$$\operatorname{Im} k(z) \geq 0, \quad z \in \mathbb{C}. \tag{J.4}$$

Relativistic point interactions concentrated at a point $y \in \mathbb{R}$ can now be constructed as follows. Define the closed, symmetric operator (cf. (I.4.1)) in $L^2(\mathbb{R}) \otimes \mathbb{C}^2$

$$\dot{D}_y = D, \qquad \mathscr{D}(\dot{D}_y) = \{g \in H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2 | g(y) = 0\}. \tag{J.5}$$

Here $g(y) = 0$ abbreviates $g_1(y) = g_2(y) = 0$ where

$$g(y) = \begin{bmatrix} g_1(y) \\ g_2(y) \end{bmatrix} \in H^{2,1}(\mathbb{R}) \otimes \mathbb{C}^2.$$

Then $\dot{D}_y$ has deficiency indices (2, 2) and hence a four-parameter family of self-adjoint extensions. Similar to our treatment of δ- and δ'-interactions for Schrödinger operators, we now select two special one-parameter families of self-adjoint extensions of $\dot{D}_y$. The first family, denoted by $D_{\alpha,y}$, is defined as

$$\begin{aligned} &D_{\alpha,y} = D, \\ &\mathscr{D}(D_{\alpha,y}) = \{g \in H^{2,1}(\mathbb{R} - \{y\}) \otimes \mathbb{C}^2 | g_1 \in AC_{\text{loc}}(\mathbb{R}), g_2 \in AC_{\text{loc}}(\mathbb{R} - \{y\}); \\ &\qquad g_2(0+) - g_2(0-) = -(i\alpha/c) g_1(0)\}, \qquad -\infty < \alpha \leq \infty. \end{aligned} \tag{J.6}$$

The second family is given by

$$\begin{aligned} &T_{\beta,y} = D, \\ &\mathscr{D}(T_{\beta,y}) = \{g \in H^{2,1}(\mathbb{R} - \{y\}) \otimes \mathbb{C}^2 | g_1 \in AC_{\text{loc}}(\mathbb{R} - \{y\}), g_2 \in AC_{\text{loc}}(\mathbb{R}); \\ &\qquad g_1(0+) - g_1(0-) = i\beta c g_2(0)\}, \qquad -\infty < \beta \leq \infty. \end{aligned} \tag{J.7}$$

Here $AC_{\text{loc}}(\Omega)$ denotes the set of locally absolutely continuous functions on $\Omega \subseteq \mathbb{R}$.

To analyze the above operators it suffices to describe their resolvents. We have

$$(D_{\alpha,y} - z)^{-1} = R_k - [\alpha/2c(2c + i\alpha\zeta)](\overline{\tilde{f}_k(\cdot - y)}, \cdot) f_k(\cdot - y), \tag{J.8}$$

$$\begin{aligned} &(T_{\beta,y} - z)^{-1} = R_k + [\beta/2(2 - i\beta c\zeta^{-1})](\overline{\tilde{g}_k(\cdot - y)}, \cdot) g_k(\cdot - y), \\ &\qquad z \in \mathbb{C} - \{(-\infty, -c^2/2] \cup [c^2/2, \infty)\}, \quad \operatorname{Im} k > 0, \end{aligned} \tag{J.9}$$

where

$$\begin{aligned} &f_k(x) = \begin{bmatrix} \zeta \\ \operatorname{sgn}(x) \end{bmatrix} e^{ik|x|}, \qquad \tilde{f}_k(x) = \begin{bmatrix} -\zeta \\ \operatorname{sgn}(x) \end{bmatrix} e^{ik|x|}, \\ &g_k(x) = \begin{bmatrix} \operatorname{sgn}(x) \\ \zeta^{-1} \end{bmatrix} e^{ik|x|}, \qquad \tilde{g}_k(x) = \begin{bmatrix} \operatorname{sgn}(x) \\ -\zeta^{-1} \end{bmatrix} e^{ik|x|}, \\ &\qquad z \in \mathbb{C} - \{(-\infty, -c^2/2] \cup [c^2/2, \infty)\}, \quad \operatorname{Im} k > 0. \end{aligned} \tag{J.10}$$

Spectral properties of $D_{\alpha,y}$ and $T_{\beta,y}$ can now be read off directly from (J.8) and (J.9). For instance, $D_{\alpha,y}$ has an eigenvalue iff $\alpha < 0$

$$\sigma_p(D_{\alpha,y}) = \begin{cases} \left\{\dfrac{c^2(4c^2 - \alpha^2)}{2(4c^2 + \alpha^2)}\right\}, & \alpha < 0, \\ \varnothing, & \alpha \geq 0, \quad \alpha = \infty, \end{cases} \tag{J.11}$$

and a resonance iff $\alpha \geq 0$ whereas $T_{\beta,y}$ has an eigenvalue iff $\beta < 0$

$$\sigma_p(T_{\beta,y}) = \begin{cases} \left\{\dfrac{c^2(\beta^2c^2-4)}{2(\beta^2c^2+4)}\right\}, & \beta < 0, \\ \varnothing, & \beta \geq 0, \quad \beta = \infty, \end{cases} \tag{J.12}$$

and a resonance iff $\beta \geq 0$. Clearly, both spectra are purely absolutely continuous in $(-\infty, -c^2/2] \cup [c^2/2, \infty)$. Given (J.8) and (J.9) the analogs of all results in Sects. I.3.1 and I.3.4 (up to (I.3.4.9)) resp. those in Ch. I.4 can now be established in a straightforward manner.

Finally, we briefly discuss the nonrelativistic limit $c \to \infty$. Applying the strategy of [202], [203], one proves that $(D_{\alpha,y} - (c^2/2) - z)^{-1}$ and $(T_{\beta,y} - (c^2/2) - z)^{-1}$, $z \in \mathbb{C} - \mathbb{R}$, are holomorphic with respect to c^{-1} in norm and that

$$\underset{c\to\infty}{\text{n-lim}}\,(D_{\alpha,y} - (c^2/2) - z)^{-1} = (-\Delta_{\alpha,y} - z)^{-1} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \qquad \alpha \in \mathbb{R}, \tag{J.13}$$

$$\underset{c\to\infty}{\text{n-lim}}\,(T_{\beta,y} - (c^2/2) - z)^{-1} = (\Xi_{\beta,y} - z)^{-1} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \qquad \beta \in \mathbb{R}, \tag{J.14}$$

In particular, the bound state energies $E_{\alpha,y}$ of $D_{\alpha,y}$, $\alpha < 0$, and $\tilde{E}_{\beta,y}$ of $T_{\beta,y}$, $\beta < 0$ (with rest energy $c^2/2$ subtracted) turn out to be holomorphic in c^{-2} around their respective nonrelativistic limits

$$\begin{aligned} E_{\alpha,y} - c^2/2 &= -(\alpha^2/4)[1 + (\alpha^2/4c^2)]^{-1}, && \alpha < 0, \\ \tilde{E}_{\beta,y} - c^2/2 &= -(4/\beta^2)[1 + (4/\beta^2c^2)]^{-1}, && \beta < 0. \end{aligned} \tag{J.15}$$

Next we quickly turn to the N-center case. Obviously, the corresponding operators are defined by

$$\begin{aligned} &D_{\alpha,Y} = D, \\ &\mathscr{D}(D_{\alpha,Y}) = \{g \in H^{2,1}(\mathbb{R} - Y) \otimes \mathbb{C}^2 \mid g_1 \in AC_{\mathrm{loc}}(\mathbb{R}), g_2 \in AC_{\mathrm{loc}}(\mathbb{R} - Y); \\ &\qquad g_2(y_j+) - g_2(y_j-) = -(i\alpha_j/c)g_1(y_j), j = 1, \ldots, N\}, \\ &\qquad \alpha = (\alpha_1, \ldots, \alpha_N), \quad -\infty < \alpha_j \leq \infty, \quad j = 1, \ldots, N, \end{aligned} \tag{J.16}$$

$$\begin{aligned} &T_{\beta,Y} = D, \\ &\mathscr{D}(T_{\beta,Y}) = \{g \in H^{2,1}(\mathbb{R} - Y) \otimes \mathbb{C}^2 \mid g_1 \in AC_{\mathrm{loc}}(\mathbb{R} - Y), g_2 \in AC_{\mathrm{loc}}(\mathbb{R}); \\ &\qquad g_1(y_j+) - g_1(y_j-) = -i\beta_j c g_2(y_j), j = 1, \ldots, N\}, \\ &\qquad \beta = (\beta_1, \ldots, \beta_N), \quad -\infty < \beta_j \leq \infty, \quad j = 1, \ldots, N, \end{aligned} \tag{J.17}$$

where $Y = \{y_1, \ldots, y_N\} \subset \mathbb{R}$. Their resolvents now read

$$(D_{\alpha,Y} - z)^{-1} = R_k + \sum_{j,j'=1}^{N} [M_{\alpha,Y}(k)]^{-1}_{jj'} (\overline{\tilde{f}_k(\cdot - y_{j'})}, \cdot) f_k(\cdot - y_j),$$
$$z \in \rho(D_{\alpha,Y}), \quad \operatorname{Im} k > 0, \tag{J.18}$$

where

$$M_{\alpha,Y}(k) = -[(4c^2/\alpha_j)\delta_{jj'} + 2ic\zeta e^{ik|y_j-y_{j'}|}]_{j,j'=1}^N \tag{J.19}$$

and

$$(T_{\beta,Y} - z)^{-1} = R_k + \sum_{j,j'=1}^N [\tilde{M}_{\beta,Y}(k)]_{jj'}^{-1}(\overline{\tilde{g}_k(\cdot - y_{j'})}, \cdot) g_k(\cdot - y_j),$$

$$z \in \rho(T_{\beta,Y}), \quad \operatorname{Im} k > 0, \tag{J.20}$$

where

$$\tilde{M}_{\beta,Y}(k) = [(4/\beta_j)\delta_{jj'} - 2ic\zeta^{-1} e^{ik|y_j-y_{j'}|}]_{j,j'=1}^N. \tag{J.21}$$

Again the analogous results of Sects. II.2.1 and II.2.4 (up to (II.2.4.7)) and Ch. II.3 can now be obtained in a straightforward manner. Obviously, also (J.13) and (J.14) trivially extend to the present situation. Hence we turn to the infinite center case. In principle, one could now follow the beginning of Sect. III.2.1 or of Ch. III.3 step by step but we prefer to proceed via the underlying difference equation scheme. In fact, due to the continuity of f_1 in the model $D_{\alpha,Y}$ and the continuity of f_2 in the model $T_{\beta,Y}$ we shall finally end up with difference equations completely analogous to those used in connection with $-\Delta_{\alpha,Y}$ and $\Xi_{\beta,Y}$.

Let $Y = \{y_j \in \mathbb{R} | j \in \mathbb{Z}\}$ be a discrete subset of $\mathbb{R}$ satisfying (III.2.1.1), $y_j < y_{j+1}$, $j \in \mathbb{Z}$, $\bigcup_{j\in\mathbb{Z}} [y_j, y_{j+1}] = \mathbb{R}$. The corresponding models are then defined by

$$D_{\alpha,Y} = D,$$

$$\mathscr{D}(D_{\alpha,Y}) = \{g \in H^{2,1}(\mathbb{R} - Y) \otimes \mathbb{C}^2 | g_1 \in AC_{\mathrm{loc}}(\mathbb{R}),\ g_2 \in AC_{\mathrm{loc}}(\mathbb{R} - Y);$$

$$g_2(y_j+) - g_2(y_j-) = -(i\alpha_j/c) g_1(y_j), j \in \mathbb{Z}\},$$

$$\alpha = \{\alpha_j\}_{j\in\mathbb{Z}}, \quad -\infty < \alpha_j \leq \infty, \quad j \in \mathbb{Z}, \tag{J.22}$$

and

$$T_{\beta,Y} = D,$$

$$\mathscr{D}(T_{\beta,Y}) = \{g \in H^{2,1}(\mathbb{R} - Y) \otimes \mathbb{C}^2 | g_1 \in AC_{\mathrm{loc}}(\mathbb{R} - Y),\ g_2 \in AC_{\mathrm{loc}}(\mathbb{R});$$

$$g_1(y_j+) - g_1(y_j-) = -i\beta_j c g_2(y_j), j \in \mathbb{Z}\},$$

$$\beta = \{\beta_j\}_{j\in\mathbb{Z}}, \quad -\infty < \beta_j \leq \infty, \quad j \in \mathbb{Z}. \tag{J.23}$$

At this point we would like to mention that the spectra of $D_{\alpha,Y}$ and $T_{\beta,Y}$ are closely related since one trivially infers that

$$[1 \otimes \sigma_2] D_{\alpha,Y} [1 \otimes \sigma_2]^{-1} = -T_{\alpha/c^2,Y}, \quad \alpha = \{\alpha_j\}_{j\in\mathbb{Z}}, \quad -\infty < \alpha_j \leq \infty, \quad j \in \mathbb{Z}, \tag{J.24}$$

where

$$\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}. \tag{J.25}$$

Following now the approach of Ch. III.3 step by step one arrives at the analog of Theorem III.3.3 and a difference equation similar to (III.3.17) resp. (III.3.20) (or the corresponding statements of Theorem III.2.1.5 and (III.2.1.48) resp. (III.2.1.49)). Since we cannot analyze these difference equations in general we only state the results in the special case where Y equals the lattice $\Lambda = a\mathbb{Z}$, $a > 0$. Then one obtains

$$M_j(k)\Phi_j(k) = \Phi_{j+1}(k), \qquad \operatorname{Im} k \geq 0, \quad k \neq m\pi/a, \quad j, m \in \mathbb{Z}, \tag{J.26}$$

where

$$\Phi_j(k) = \begin{bmatrix} \psi_1(k, y_j) \\ \psi_1(k, y_{j-1}) \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{J.27}$$

and $M_j(k) = M_j^D(k)$ for the operator $D_{\alpha,\Lambda}$ where

$$M_j^D(k) = \begin{bmatrix} (\alpha_j/c)\zeta \sin(ka) + 2\cos(ka) & -1 \\ 1 & 0 \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{J.28}$$

$$(D_{\alpha,\Lambda}\psi)(k, x) = E\psi(k, x), \qquad x \in \mathbb{R} - \Lambda, \qquad \psi(k, x) = \begin{bmatrix} \psi_1(k, x) \\ \psi_2(k, x) \end{bmatrix},$$

$$\psi_1(k, aj+) = \psi_1(k, aj-), \qquad \psi_2(k, aj+) - \psi_2(k, aj-) = -(i\alpha_j/c)\psi_1(k, aj),$$
$$j \in \mathbb{Z}, \quad E \in \mathbb{R}, \quad \operatorname{Im} k \geq 0 \tag{J.29}$$

in the case of model $D_{\alpha,\Lambda}$ and where

$$\Phi_j(k) = \begin{bmatrix} \psi_2(k, y_j) \\ \psi_2(k, y_{j-1}) \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{J.30}$$

and $M_j(k) = M_j^T(k)$ for the operator $T_{\beta,\Lambda}$ where

$$M_j^T(k) = \begin{bmatrix} -\beta_j c\zeta^{-1} \sin(ka) + 2\cos(ka) & -1 \\ 1 & 0 \end{bmatrix}, \qquad \operatorname{Im} k \geq 0, \quad j \in \mathbb{Z}, \tag{J.31}$$

$$(T_{\beta,\Lambda}\psi)(k, x) = E\psi(k, x), \qquad x \in \mathbb{R} - \Lambda, \qquad \psi(k, x) = \begin{bmatrix} \psi_1(k, x) \\ \psi_2(k, x) \end{bmatrix},$$

$$\psi_2(k, aj+) = \psi_2(k, aj-), \qquad \psi_1(k, aj+) - \psi_1(k, aj-) = i\beta_j c\psi_2(k, aj),$$
$$j \in \mathbb{Z}, \quad E \in \mathbb{R}, \quad \operatorname{Im} k \geq 0, \tag{J.32}$$

in the case of model $T_{\beta,\Lambda}$. Explicitly, the two difference equations read

$$\begin{aligned} \psi_{j+1}(k) + \psi_{j-1}(k) &= \{(\alpha_j/c)\zeta \sin(ka) + 2\cos(ka)\}\psi_j(k), \\ \psi_j(k) &= \psi_1(k, aj), \qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m/a, \quad j, m \in \mathbb{Z}, \end{aligned} \tag{J.33}$$

in the case of $D_{\alpha,\Lambda}$ and

$$\begin{aligned} \psi_{j+1}(k) + \psi_{j-1}(k) &= \{-\beta_j c\zeta^{-1} \sin(ka) + 2\cos(ka)\}\psi_j(k), \\ \psi_j(k) &= \psi_2(k, aj), \qquad \operatorname{Im} k \geq 0, \quad k \neq \pi m/a, \quad j, m \in \mathbb{Z}, \end{aligned} \tag{J.34}$$

in the case of $T_{\beta,\Lambda}$. Thus we get completely analogous results to (III.2.1.54), (III.2.1.55) for $-\Delta_{\alpha,\Lambda}$ and to (III.3.23) and (III.3.24) for $\Xi_{\beta,\Lambda}$.

Next we analyze the energy band spectra of $D_{\alpha,\Lambda}$ and $T_{\beta,\Lambda}$ in the periodic case where $\alpha_j = \alpha$ (resp. $\beta_j = \beta$), $j \in \mathbb{Z}$. First, we introduce the reduced operators $D_{\alpha,\Lambda}(\theta)$, $T_{\beta,\Lambda}(\theta)$ in $L^2((-a/2, a/2)) \otimes \mathbb{C}^2$ by

$$\begin{aligned} D_{\alpha,\Lambda}(\theta) &= D, \\ \mathscr{D}(D_{\alpha,\Lambda}(\theta)) &= \{g(\theta) \in H^{2,1}((-a/2, a/2) - \{0\}) \otimes \mathbb{C}^2 | \\ &\qquad g_n(\theta, -a/2+) = e^{i\theta a} g_n(\theta, a/2-), n = 1,2; g_1(\theta, 0+) = g_1(\theta, 0-), \\ &\qquad g_2(\theta, 0+) - g_2(\theta, 0-) = -(i\alpha/c) g_2(\theta, 0)\}, \\ &\qquad\qquad -\infty < \alpha \le \infty, \quad \theta \in [-b/2, b/2), \end{aligned} \tag{J.35}$$

and

$$\begin{aligned} T_{\beta,\Lambda}(\theta) &= D, \\ \mathscr{D}(T_{\beta,\Lambda}(\theta)) &= \{g(\theta) \in H^{2,1}((-a/2, a/2) - \{0\}) \otimes \mathbb{C}^2 | \\ &\qquad g_n(\theta, -a/2+) = e^{i\theta a} g_n(\theta, a/2-), n = 1,2; g_2(\theta, 0+) = g_2(\theta, 0-), \\ &\qquad g_1(\theta, 0+) - g_1(\theta, 0-) = i\beta c g_2(\theta, 0)\}, \\ &\qquad\qquad -\infty < \beta \le \infty, \quad \theta \in [-b/2, b/2). \end{aligned} \tag{J.36}$$

Then

$$\begin{aligned} \tilde{\mathscr{U}} D_{\alpha,\Lambda} \tilde{\mathscr{U}}^{-1} &= \int_{[-b/2, b/2)}^{\oplus} \frac{d\theta}{b} D_{\alpha,\Lambda}(\theta), \\ \tilde{\mathscr{U}} T_{\beta,\Lambda} \tilde{\mathscr{U}}^{-1} &= \int_{[-b/2, b/2)}^{\oplus} \frac{d\theta}{b} T_{\beta,\Lambda}(\theta), \end{aligned} \tag{J.37}$$

in analogy to (III.2.3.27) and (III.3.43) where $\tilde{\mathscr{U}}$ is now the analog of (III.2.3.8), mapping $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ onto $L^2(\hat{\Lambda}, b^{-1}\, d\theta; L^2([-a/2, a/2)) \otimes \mathbb{C}^2)$.

Spectral properties of $D_{\alpha,\Lambda}(\theta)$ are summarized in

Theorem J.1. *Let $-\infty < \alpha \le \infty$, $\theta \in [-b/2, b/2)$. Then the essential spectrum of $D_{\alpha,\Lambda}(\theta)$ is empty*

$$\sigma_{\text{ess}}(D_{\alpha,\Lambda}(\theta)) = \varnothing \tag{J.38}$$

and thus the spectrum of $D_{\alpha,\Lambda}(\theta)$ is purely discrete. In particular, its eigenvalues $E_m^{\alpha,\Lambda}(\theta)$, $m \in \mathbb{Z} - \{0\}$, are given by

$$\begin{aligned} E_m^{\alpha,\Lambda}(\theta) &= \operatorname{sgn}(m) |[k_m^{\alpha,\Lambda}(\theta)]^2 c^2 + (c^4/4)|^{1/2}, \qquad m \in \mathbb{Z} - \{0, 1\}, \\ E_1^{\alpha,\Lambda}(\theta) &= [[k_1^{\alpha,\Lambda}(\theta)]^2 c^2 + (c^4/4)]^{1/2}, \end{aligned} \tag{J.39}$$

where for $m = 1$ the branch of the square root to be chosen in (J.39) *depends on α and θ and where $k_m^{\alpha,\Lambda}(\theta)$, $m \in \mathbb{Z} - \{0\}$, ordered with respect to their* *absolute values, are solutions of*

$$\cos(\theta a) = \cos(ka) + [\alpha\xi(k)/2c]\sin(ka), \qquad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \tag{J.40}$$

with

$$\xi(k) = \zeta(E) = \{\operatorname{sgn}(E)[k^2c^2 + (c^4/4)]^{1/2} + (c^2/2)\}/ck, \tag{J.41}$$

$$k = k(E) = \begin{cases} |E^2 - (c^4/4)|^{1/2}, & |E| \geq c^2/2, \\ i|(c^4/4) - E^2|^{1/2}, & |E| \leq c^2/2. \end{cases} \tag{J.42}$$

For $\alpha \in \mathbb{R} - \{0\}$, except for $\alpha = -ac^2$, $m = 1$ and $\theta = 0$, the eigenvalues $E_m^{\alpha,\Lambda}(\theta)$ are simple. If $\alpha = -ac^2$, then $E_1^{-ac^2,\Lambda}(0)$ has multiplicity two.

Let $\alpha > 0$. For $E \geq 0$ we obtain

$$\begin{aligned} c^2/2 &< E_1^{\alpha,\Lambda}(0) < E_1^{\alpha,\Lambda}(-b/2) = [(\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &< E_2^{\alpha,\Lambda}(-b/2) < E_2(0) = [(4\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &< E_3^{\alpha,\Lambda}(0) < E_3^{\alpha,\Lambda}(-b/2) = [(9\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &< E_4^{\alpha,\Lambda}(0) < \cdots . \end{aligned} \tag{J.43}$$

For $E \leq 0$ we get

$$\begin{aligned} E_{-1}^{\alpha,\Lambda}(0) &= -c^2/2 > E_{-1}^{\alpha,\Lambda}(-b/2) > E_{-2}^{\alpha,\Lambda}(-b/2) = -[(\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &> E_{-2}^{\alpha,\Lambda}(0) > E_{-3}^{\alpha,\Lambda}(0) = -[(4\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &> E_{-3}^{\alpha,\Lambda}(-b/2) > E_{-4}^{\alpha,\Lambda}(-b/2) = -[(9\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &> E_{-4}(0) > \cdots . \end{aligned} \tag{J.44}$$

In addition,

$$\sigma(D_{\alpha,\Lambda}(\theta)) \cap (-c^2/2, c^2/2) = \varnothing, \qquad \alpha > 0, \quad \theta \in [-b/2, b/2). \tag{J.45}$$

Next let $\alpha < 0$. For $E \geq -c^2/2$ we obtain

$$\begin{aligned} &E_1^{\alpha,\Lambda}(0) < E_1^{\alpha,\Lambda}(-b/2) < E_2^{\alpha,\Lambda}(-b/2) = [(\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &\qquad < E_2^{\alpha,\Lambda}(0) < E_3^{\alpha,\Lambda}(0) = [(4\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &\qquad < E_3^{\alpha,\Lambda}(-b/2) < E_4^{\alpha,\Lambda}(-b/2) = [(9\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\ &\qquad < E_4^{\alpha,\Lambda}(0) < \cdots , \\ &-c^2/2 \leq E_1^{\alpha,\Lambda}(0) < c^2/2, \quad \alpha \in \mathbb{R}, \\ &E_1^{-(2c)\tanh(ac/4),\Lambda}(0) = 0, \qquad E_1^{\alpha,\Lambda}(0) = -c^2/2, \quad \alpha \leq -ac^2, \\ &-c^2/2 < E_1^{\alpha,\Lambda}(-b/2) < [(\pi^2c^2/a^2) + (c^4/4)]^{1/2}, \qquad \alpha \in \mathbb{R}, \\ &E_1^{-4/a,\Lambda}(-b/2) = c^2/2, \qquad E_1^{-(2c)\coth(ac/4),\Lambda}(-b/2) = 0, \\ &E_1^{\alpha,\Lambda}(-b/2) \xrightarrow[\alpha \to -\infty]{} -c^2/2. \end{aligned} \tag{J.46}$$

For $E \leq -c^2/2$ *we get*

$$
\begin{aligned}
E_{-1}^{\alpha,\Lambda}(0) > E_{-1}^{\alpha,\Lambda}(-b/2) &= -[(\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\
> E_{-2}^{\alpha,\Lambda}(-b/2) > E_{-2}^{\alpha,\Lambda}(0) &= -[(4\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\
> E_{-3}^{\alpha,\Lambda}(0) > E_{-3}^{\alpha,\Lambda}(-b/2) &= -[(9\pi^2c^2/a^2) + (c^4/4)]^{1/2} \\
> E_{-4}^{\alpha,\Lambda}(-b/2) > \cdots,&
\end{aligned}
$$

$$
E_1^{\alpha,\Lambda}(0)\begin{cases} = -c^2/2, & -ac^2 \leq \alpha < 0, \\ < -c^2/2, & \alpha < -ac^2. \end{cases} \tag{J.47}
$$

All nonconstant eigenvalues $E_m^{\alpha,\Lambda}(\theta)$, $\theta \in [-b/2, b/2)$, $m \in \mathbb{Z} - \{0\}$, *are strictly increasing with respect to* $\alpha \in \mathbb{R}$. *For* $\alpha = 0$ *the eigenvalues are given by*

$$
E_{m\pm}^{0,\Lambda}(\theta) = \pm\{[\theta + 2\,\mathrm{sgn}(m)||m| - 1|\pi a^{-1}]^2c^2 + (c^4/4)\}^{1/2},
$$

$$
m \in \mathbb{Z} - \{0\}, \quad \theta \in [-b/2, 0]. \tag{J.48}
$$

They are only degenerate for $\theta = -b/2, m \in \mathbb{Z} - \{0\}$ *and* $\theta = 0, |m| \geq 2$.

PROOF. Since practically all arguments parallel those used in the proof of Theorem III.2.3.1 and Theorem III.3.4, respectively, we only concentrate on the derivation of (J.40)–(J.47). Using the ansatz (III.3.35) in (J.33) yields (J.40). Concerning (J.41) and (J.42) we used the resolvent (J.4). For $|E| \geq c^2/2$ and $\theta = 0, -b/2$, (J.40) becomes

$$
\begin{aligned}
&\sin(ka/2) = 0 \quad \text{or} \quad \cot(ka/2) = 2c/\alpha\xi(k) && \text{for} \quad \theta = 0, \\
&\sin[(ka + \pi)/2] = 0 \quad \text{or} \quad \cot[(ka + \pi)/2] = 2c/\alpha\xi(k) && \text{for} \quad \theta = -b/2; \\
& && k \geq 0.
\end{aligned} \tag{J.49}
$$

Since

$$
\begin{aligned}
&1/\xi(k) = kc/\{[k^2c^2 + (c^4/4)]^{1/2} + (c^2/2)\} \in [0, 1), && E \geq c^2/2, \\
&\xi(k) = \{-[k^2c^2 + (c^4/4)]^{1/2} + (c^2/2)\}/kc \in (-1, 0], && E \leq -c^2/2, \\
&\xi'(k) < 0, \qquad k > 0, &&
\end{aligned} \tag{J.50}
$$

equations (J.43) and (J.44) follow immediately in the case $\alpha > 0$.

For $E \in [-c^2/2, c^2/2]$ and $\theta = 0, -b/2$, (J.40) becomes

$$
\pm 1 = \cosh(\kappa a) + [\alpha\eta(\kappa)/2c]\sinh(\kappa a), \qquad \theta = \begin{cases} 0, \\ -b/2, \end{cases} \tag{J.51}
$$

where

$$
\begin{aligned}
&\kappa = -ik = [(c^4/4) - E^2]^{1/2}/c \in [0, c/2], \\
&1/\eta(\kappa) = 1/i\xi(i\kappa) = \kappa c/\{[(c^4/4) - \kappa^2c^2]^{1/2} + (c^2/2)\} \in [0, 1], && E \in [0, c^2/2], \\
&\eta(\kappa) = i\xi(i\kappa) = \{-[(c^4/4) - \kappa^2c^2]^{1/2} + (c^2/2)\}/\kappa c \in [0, 1], && E \in [-c^2/2, 0].
\end{aligned} \tag{J.52}
$$

Clearly, (J.51) has no solutions for $\alpha > 0$ implying (J.45). Before we turn to the case

$\alpha < 0$ we first prove that $D_{\alpha,\Lambda}(\theta)$, $\alpha \in \mathbb{R}$, has at most one eigenvalue in $(-c^2/2, c^2/2)$. For that purpose we define the closed, symmetric operator $\dot{D}_\theta$ in $L^2((-a/2, a/2)) \otimes \mathbb{C}^2$ by

$$\dot{D}_\theta = D,$$

$$\mathscr{D}(\dot{D}_\theta) = \{g \in H^{2,1}((-a/2, a/2)) \otimes \mathbb{C}^2 | g_n(-a/2+) = e^{i\theta a} g_n(a/2-), n = 1, 2, g_2(0) = 0\},$$
$$\theta \in [-b/2, b/2). \quad \text{(J.53)}$$

By inspection $\operatorname{def}(\dot{D}_\theta) = (1, 1)$, $\theta \in [-b/2, b/2)$. Since both $D_{\alpha,\Lambda}(\theta)$ and $D_{0,\Lambda}(\theta)$ are self-adjoint extensions of $\dot{D}_\theta$, and $D_{0,\Lambda}(\theta)$ (the decomposed free Dirac operator) obviously has no eigenvalues in $(-c^2/2, c^2/2)$ for all $\theta \in [-b/2, b/2)$, $D_{\alpha,\Lambda}(\theta)$, $\alpha \in \mathbb{R}$, $\theta \in [-b/2, b/2)$, can have at most one eigenvalue in $(-c^2/2, c^2/2)$ by Corollary 1 of [494], p. 246.

Now we treat the case $\alpha < 0$. Since the only nontrivial computations concern $E_1^{\alpha,\Lambda}(\theta)$ and $E_1^{\alpha,\Lambda}(-b/2)$ we confine ourselves to a detailed discussion of the latter. We start with $E_1^{\alpha,\Lambda}(-b/2)$. For $E \geq c^2/2$, the first solution k_1 of

$$\cot[(ka + \pi)/2] = 2c/\alpha\xi(k), \qquad k \geq 0, \quad \text{(J.54)}$$

(cf. (J.49)) is strictly decreasing from $k_1 = \pi/a$ for $\alpha = 0$ to $k_1 = 0$ for $\alpha = -4/a$. For $E \in [-c^2/2, c^2/2]$ we have to analyze (J.51) and (J.52) in more detail. First of all, (J.51) is equivalent to

$$\begin{aligned} &\coth(\kappa a/2) = 2c/|\alpha|\eta(\kappa) \qquad \text{for} \quad \theta = 0, \\ &\tanh(\kappa a/2) = 2c/|\alpha|\eta(\kappa) \qquad \text{for} \quad \theta = -b/2; \quad E \in [-c^2/2, c^2/2], \end{aligned} \quad \text{(J.55)}$$

by taking into account that for $\theta = 0$, $\kappa = 0$ is always a solution of (J.51) for all $\alpha \in \mathbb{R}$ whereas for $\theta = -b/2$, $\kappa = 0$ is a solution of (J.51) iff $\alpha = -4/a$. Moreover, we note

$$\eta'(\kappa)\begin{cases} <0, & E > 0, \\ >0, & E < 0, \end{cases}$$

$$\eta''(\kappa)\begin{cases} >0, & 0 < \kappa < \sqrt{3}c/4, \\ <0, & \sqrt{3}c/4 < \kappa < c/2, \end{cases} \qquad \eta''(\sqrt{3}c/4) = 0, \quad E > 0,$$

$$\eta''(\kappa) > 0, \qquad E < 0. \quad \text{(J.56)}$$

Now we continue our discussion of $E_1^{\alpha,\Lambda}(-b/2)$, $\alpha < 0$. First, we prove that (J.55) for $\theta = -b/2$ has no solutions for $-4/a < \alpha < 0$. This follows from

$$2c/|\alpha|\eta(\kappa) > 2ac/4\eta(\kappa) > \kappa a/2 > \tanh(\kappa a/2). \quad \text{(J.57)}$$

Next we prove that (J.55) for $\theta = -b/2$ and $E \in (0, c^2/2)$ has no solutions for $\alpha < -(2c)\coth(ac/4)$. In fact, by the monotonicity with respect to $|\alpha|$ we only need to prove that

$$\tanh(\kappa a/2) = 2c/|\alpha_0|\eta(\kappa), \qquad E \in (0, c^2/2), \qquad \alpha_0 = -(2c)\coth(ac/4) \quad \text{(J.58)}$$

has as only solutions $\kappa = 0$ and $\kappa = c/2$. Since $[x^{-1}\tanh(x)]' < 0$ for $x > 0$ we get indeed

$$\begin{aligned} \tanh(\kappa a/2) &> (\kappa/2c)\tanh(ac/4) \\ &> (\kappa/2c)\{1 + [1 - (4\kappa^2/c^2)]^{1/2}\}^{-1}\tanh(ac/4) = 2c/|\alpha_0|\eta(\kappa), \end{aligned}$$
$$0 < \kappa < c/2. \quad \text{(J.59)}$$

In order to discuss the case $E \to 0$ we note

$$\eta(\kappa) \underset{\kappa \to c/2-}{=} 1 + \operatorname{sgn}(E) c^{3/2}[(c/2) - \kappa]^{1/2} + O([(c/2) - \kappa]). \tag{J.60}$$

Inserting (J.60) into (J.51) for $\theta = -b/2$ shows that

$$\{\cosh(\kappa a) + [\alpha\eta(\kappa)/2c] \sinh(\kappa a)\}|_{\alpha = -(2c)\coth(ac/4)}$$
$$\underset{\kappa \to c/2-}{=} -1 - \operatorname{sgn}(E) \coth(ac/4) c^{3/2}[(c/2) - \kappa]^{1/2} + O([(c/2) - \kappa]). \tag{J.61}$$

Hence $(0, \varepsilon) \cap \sigma(D_{\alpha_0, \Lambda}) = \varnothing$, $[-\varepsilon, 0] \subset \sigma(D_{\alpha_0, \Lambda})$ for $\varepsilon > 0$ small enough, and $\alpha_0 = -(2c)\coth(ac/4)$. For $E \in [0, c^2/2]$ and $-(2c)\coth(ac/4) \le \alpha \le -4/a$, (J.55) for $\theta = -b/2$ has a unique solution as can be seen as follows. Near $\kappa = 0$ we obviously get the inequality

$$\tanh(\kappa a/2) > 2c/|\alpha| \eta(\kappa), \qquad \kappa > 0 \text{ small enough}, \tag{J.62}$$

whereas for $\kappa \to c/2-$ we have

$$\tanh(\kappa a/2) < 2c/|\alpha| \eta(\kappa), \qquad [(c/2) - \kappa] > 0 \text{ small enough}. \tag{J.63}$$

By the continuity properties of η there exists at least one solution of (J.55) for $\theta = -b/2$. But by the arguments following (J.53) there exists at most one solution proving the above claim. For $E \in (-c^2/2, 0]$ and $\alpha \le -(2c)\coth(ac/4)$, (J.55) for $\theta = -b/2$ has a unique solution since $2c/|\alpha|\eta(\kappa)$ is strictly decreasing from $+\infty$ to $2c/|\alpha|$ and $\tanh(\kappa a/2)$ is strictly increasing from 0 to $\tanh(ac/4)$ as κ varies from 0 to $c/2$. Clearly, this solution tends to zero as $\alpha \to -\infty$. This completes the discussion of $E_1^{\alpha,\Lambda}(-b/2)$. It remains to treat $E_1^{\alpha,\Lambda}(0)$. For $E \in [0, c^2/2)$ and $-(2c)\tanh(ac/4) \le \alpha < 0$, (J.55) for $\theta = 0$ has a unique solution since $\coth(\kappa a/2)$ is strictly decreasing from $+\infty$ to $\coth(ac/4)$ and $2c/|\alpha|\eta(\kappa)$ is strictly increasing from 0 to $2c/|\alpha|$ as κ varies from 0 to $c/2$. Inserting (J.60) into (J.51) for $\theta = 0$ yields

$$\{\cosh(\kappa a) + [\alpha\eta(\kappa)/2c] \sinh(\kappa a)\}|_{\alpha = -(2c)\tanh(ac/4)}$$
$$\underset{\kappa \to c/2-}{=} 1 - \operatorname{sgn}(E) \tanh(ac/4) c^{3/2}[(c/2) - \kappa]^{1/2} + O([(c/2) - \kappa]). \tag{J.64}$$

Hence $(-\varepsilon, 0) \cap \sigma(D_{\alpha_1, \Lambda}) = \varnothing$, $[0, \varepsilon] \subset \sigma(D_{\alpha_1, \Lambda})$ for $\varepsilon > 0$ small enough and $\alpha_1 = -(2c)\tanh(ac/4)$. For $E \in [-c^2/2, 0]$ and $-ac^2 \le \alpha \le -(2c)\tanh(ac/4)$, (J.55) for $\theta = 0$ has a unique solution by the following reasoning. Near $\kappa = 0$ we infer that

$$\coth(\kappa a/2) < 2c/|\alpha| \eta(\kappa), \qquad \kappa > 0 \text{ small enough}, \tag{J.65}$$

whereas for $\kappa \to c/2-$ we get

$$\coth(\kappa a/2) > 2c/|\alpha| \eta(\kappa), \qquad [(c/2) - \kappa] > 0 \text{ small enough}. \tag{J.66}$$

By the continuity properties of η we obtain at least one solution of (J.55) for $\theta = 0$. Again by the arguments following (J.53) this solution is unique. Since for $\theta = 0$, $\kappa = 0$ is a solution of (J.51) for all $\alpha \in \mathbb{R}$ the proof is complete. ∎

The spectral properties of $T_{\beta,\Lambda}(\theta)$ now can be derived from Theorem J.1 since (cf. (J.24))

$$[1 \otimes \sigma_2] D_{\alpha,\Lambda}(\theta) [1 \otimes \sigma_2]^{-1} = -T_{\alpha/c^2,\Lambda}(\theta),$$
$$-\infty < \alpha \le \infty, \quad \theta \in [-b/2, b/2). \tag{J.67}$$

Applying now (J.37) we get

Theorem J.2. *Let $\alpha \in \mathbb{R}$ and $\Lambda = a\mathbb{Z}$, $a > 0$. Then $D_{\alpha,\Lambda}$ has purely absolutely continuous spectrum*

$$\sigma(D_{\alpha,\Lambda}) = \sigma_{ac}(D_{\alpha,\Lambda}) = \bigcup_{m \in \mathbb{Z}-\{0\}} [a_m^{\alpha,\Lambda}, b_m^{\alpha,\Lambda}],$$

$$a_m^{\alpha,\Lambda} < b_m^{\alpha,\Lambda} \leq a_{m+1}^{\alpha,\Lambda}, \quad a_{-m}^{\alpha,\Lambda} > b_{-m}^{\alpha,\Lambda} \geq a_{-(m+1)}^{\alpha,\Lambda}, \quad m \in \mathbb{N},$$

$$\sigma_{sc}(D_{\alpha,\Lambda}) = \varnothing, \quad \sigma_p(D_{\alpha,\Lambda}) = \varnothing. \tag{J.68}$$

Here for $\alpha > 0$

$$a_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(0), & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(-b/2), & m \text{ even}, \qquad m \in \mathbb{N}, \end{cases} \tag{J.69}$$

$$a_m^{\alpha,\Lambda} > [(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, \qquad m \in \mathbb{N},$$

$$b_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(-b/2) = [(m^2\pi^2c^2/a^2) + (c^4/4)]^{1/2}, & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(0) \quad\;\; = [(m^2\pi^2c^2/a^2) + (c^4/4)]^{1/2}, & m \text{ even}, \quad m \in \mathbb{N}, \end{cases}$$

$$a_{-m}^{\alpha,\Lambda} = \begin{cases} E_{-m}^{\alpha,\Lambda}(0) \quad\;\; = -[(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, & m \text{ odd}, \\ E_{-m}^{\alpha,\Lambda}(-b/2) = -[(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, & m \text{ even}, \ m \in \mathbb{N}, \end{cases}$$

$$b_{-m}^{\alpha,\Lambda} = \begin{cases} E_{-m}^{\alpha,\Lambda}(-b/2), & m \text{ odd}, \\ E_{-m}^{\alpha,\Lambda}(0), & m \text{ even}, \qquad m \in \mathbb{N}, \end{cases} \tag{J.70}$$

$$b_{-m}^{\alpha,\Lambda} < -[(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, \qquad m \in \mathbb{N}.$$

For $\alpha < 0$

$$-c^2/2 \leq a_1^{\alpha,\Lambda} = E_1^{\alpha,\Lambda}(0) < c^2/2,$$

$$a_1^{\alpha,\Lambda} = -c^2/2, \qquad \alpha \leq -ac^2, \qquad a_1^{-(2c)\tanh(ac/4),\Lambda} = 0,$$

$$a_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(0) \quad\;\; = [(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(-b/2) = [(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, & m \text{ even}, \end{cases}$$

$$m = 2, 3, 4, \ldots,$$

$$-c^2/2 < b_1^{\alpha,\Lambda} = E_1^{\alpha,\Lambda}(-b/2) < [(\pi^2c^2/a^2) + (c^4/4)]^{1/2},$$

$$b_1^{-4/a,\Lambda} = c^2/2, \qquad b_1^{-(2c)\coth(ac/4),\Lambda} = 0, \tag{J.71}$$

$$b_1^{\alpha,\Lambda} \xrightarrow[\alpha \to -\infty]{} -c^2/2,$$

$$b_m^{\alpha,\Lambda} = \begin{cases} E_m^{\alpha,\Lambda}(-b/2), & m \text{ odd}, \\ E_m^{\alpha,\Lambda}(0), & m \text{ even}, \qquad m \in \mathbb{N}, \end{cases}$$

$$b_m^{\alpha,\Lambda} > [(m-1)^2\pi^2c^2a^{-2} + (c^4/4)]^{1/2}, \qquad m = 2, 3, 4, \ldots,$$

$$a_{-1}^{\alpha,\Lambda} = E_{-1}^{\alpha,\Lambda}(0) \begin{cases} = -c^2/2, & -ac^2 \leq \alpha < 0, \\ < -c^2/2, & \alpha < -ac^2, \end{cases} \tag{J.72}$$

$$a_{-m}^{\alpha,\Lambda} = \begin{cases} E_{-m}^{\alpha,\Lambda}(0), & m \text{ odd}, \\ E_{-m}^{\alpha,\Lambda}(-b/2), & m \text{ even}, \qquad m \in \mathbb{N}, \end{cases}$$

$$a_{-m}^{\alpha,\Lambda} > -[(m^2\pi^2c^2/a^2) + (c^4/4)]^{1/2}, \qquad m \in \mathbb{N},$$

$$b_{-m}^{\alpha,\Lambda} = \begin{cases} E_{-m}^{\alpha,\Lambda}(-b/2) = -[(m^2\pi^2c^2/a^2) + (c^4/4)]^{1/2}, & m \text{ odd}, \\ E_{-m}^{\alpha,\Lambda}(0) \quad = -[(m^2\pi^2c^2/a^2) + (c^4/4)]^{1/2}, & m \text{ even}, \end{cases} \qquad m \in \mathbb{N}.$$

For $\alpha \in \mathbb{R} - \{0\}$, $D_{\alpha,\Lambda}$ has infinitely many gaps in its spectrum. Except for $\alpha = -ac^2$, all possible gaps do actually occur. Only for $\alpha = -ac^2$ one gap closes at $E = -c^2/2$ since $D_{-ac^2,\Lambda}(0)$ has $-c^2/2$ as an eigenvalue of multiplicity two. For $\alpha = 0$, $D_{0,\Lambda}$ equals the free Dirac operator D_0 in (J.1) *with spectrum*

$$\sigma(D_0) = (-\infty, -c^2/2] \cup [c^2/2, \infty) \tag{J.73}$$

and due to the degeneracy of $E_m^{0,\Lambda}(0)$, $|m| \geq 2$, and $E_m^{0,\Lambda}(-b/2)$, $m \in \mathbb{Z} - \{0\}$, all gaps in $\mathbb{R} - (-c^2/2, c^2/2)$ close. Furthermore, we note a strict monotonicity of $\sigma(D_{\alpha,\Lambda})$ with respect to α (being a consequence of the monotonicity of $E_m^{\alpha,\Lambda}(0)$, $E_m^{\alpha,\Lambda}(-b/2)$, $m \in \mathbb{Z} - \{0\}$, with respect to α as mentioned in Theorem J.1)

$$\begin{aligned} &\sigma(D_{\alpha,\Lambda}) \subset \sigma(D_{\alpha',\Lambda}), && 0 \leq \alpha' < \alpha, \\ &\sigma(D_{\alpha,\Lambda}) \supset \sigma(D_{\alpha',\Lambda}), && -\infty < \alpha' < \alpha \leq -ac^2. \end{aligned} \tag{J.74}$$

Since (J.24) obviously applies in the present special case of periodicity, the spectrum of $T_{\beta,\Lambda}$ immediately follows from Theorem J.2.

Following [116] one easily proves that $(D_{\alpha,\Lambda} - (c^2/2) - z)^{-1}$ and $(T_{\beta,\Lambda} - (c^2/2) - z)^{-1}$, $z \in C - \mathbb{R}$, are holomorphic with respect to c^{-1} in norm and that

$$\begin{aligned} &\operatorname*{n-lim}_{c\to\infty} (D_{\alpha,\Lambda} - (c^2/2) - z)^{-1} = (-\Delta_{\alpha,\Lambda} - z)^{-1} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, && \alpha \in \mathbb{R}, \\ &\operatorname*{n-lim}_{c\to\infty} (T_{\beta,\Lambda} - (c^2/2) - z)^{-1} = (\Xi_{\beta,\Lambda} - z)^{-1} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, && \beta \in \mathbb{R}. \end{aligned} \tag{J.75}$$

Moreover, first-order relativistic corrections of energy bands with respect to c^{-2} can be explicitly computed since $E_m^{\alpha,\Lambda}(\theta) - (c^2/2)$, $E_m^{\beta,\Lambda}(\theta) - (c^2/2)$, $\theta \in [-b/2, b/2)$, $m \in \mathbb{N}$, turn out to be holomorphic in c^{-2} around their nonrelativistic limits. In particular, the discriminant (J.40) and its analog for $T_{\beta,\Lambda}(\theta)$,

$$\cos(\theta a) = \cos(ka) - [\beta c/2\xi(k)] \sin(ka), \qquad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k \geq 0, \tag{J.76}$$

are easily seen to reproduce (III.2.3.16) and (III.3.29) as $c \to \infty$.

At this point we stop our analysis of relativistic point interactions in one dimension. In fact, since the difference equations for $D_{\alpha,Y}$ and $T_{\beta,Y}$ are of the same type as for $-\Delta_{\alpha,Y}$ and $\Xi_{\beta,Y}$ all results of Sects. III.2.1, III.2.3, III.2.4, III.2.6, and Ch. III.3 extend to the present case. Explicitly, we mention that the density of states (cf. (III.2.3.46) and (III.3.51)), the Saxon and Hutner conjecture (cf. Theorems III.2.3.6 and III.3.5), half-crystals, defects, and impurity scattering can now be treated by the same methods. Moreover, due to (J.42) spectral results for $T_{\beta,Y}$ immediately follow from that of $D_{\alpha,Y}$.

Notes

The entire material of this appendix is taken from Gesztesy and Šeba [210].

Another type of self-adjoint extensions of $\dot{D}_y$ has been discussed extensively in the literature. Its boundary conditions read, e.g., in the case of a discrete subset $Y \subset \mathbb{R}$ (as in (J.22) and (J.23))

$$\begin{aligned} g_1(y_j+) &= \cos(\gamma_j)g_1(y_j-) - i\sin(\gamma_j)g_2(y_j-), \\ g_2(y_j+) &= \cos(\gamma_j)g_2(y_j-) - i\sin(\gamma_j)g_1(y_j-), \qquad \gamma_j \in \mathbb{R}, \quad j \in \mathbb{Z}. \end{aligned}$$

Since in this case no linear combination of g_1 and g_2 turns out to be continuous at $y_j \in Y, j \in \mathbb{Z}$, our difference equation approach does not apply. Nevertheless this model can be analyzed directly. In the finite center case this type of model has been discussed in [232], [318], the purely periodic case in [51], [139], [175], [213], [421], [454], [456], [465], [469], the diatomic case in [421], [457], impurity states in [89], [139] and half-crystals and surface states in [138], [175], [400a], [425], [426], [454], [466]. The Saxon and Hutner conjecture in the special case $N = 2$ for this model has been proved in [465].

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