Introduction

In this monograph we study systematically certain classes of perturbations of given self–adjoint operators in Hilbert spaces. As main examples we consider second order differential operators in L^2-spaces perturbed by finite or infinite rank operators, respectively by certain generalized 'interaction terms'. Typical results concern spectral properties and scattering quantities. The operators we discuss include as special cases Hamiltonians with 'point interactions', i.e., interactions involving potentials of the δ, respectively δ'-type supported by a (finite or infinite) set of isolated points or suitable lower dimensional hypersurfaces. Such Hamiltonians occur, e.g., in the description of quantum mechanical systems in solid state physics, atomic and nuclear physics as well as in the description of electromagnetic phenomena, in the modelling of certain related chemical and biological phenomena, and in the study of quantum chaotic systems.

Concerning these 'point interaction models', in the last decade two specific monographs have appeared along with a few proceedings, books and specialized papers. One of the main aims of the present book is to present a natural continuation of the previous work [39], much in the same rigorous mathematical spirit, and covering some of the developments which occurred after the appearance of [39] (and its Russian improved version [40]). Our present book extends the analysis of [39] (and [40]) in two directions. On one hand we look at the operators discussed in [39] as special cases of a general theory of (singular) perturbations of (differential) operators. On the other hand we present results on specific perturbations of operators, described much in the same spirit of [39]. Concrete spectral properties of the operators are involved (from control over eigenvalues and eigenfunctions to scattering theory). Our discussion includes in particular the case of 'generalized point interactions', of n-th order operators in one dimension, and certain many-body (multiparticle) problems with 'delta interactions', all cases not discussed in [39] and [40].

In the books [39, 40, 255] models of quantum Hamiltonians with point interactions are considered, with special emphasis on the one–body problem with interaction concentrated at many fixed centers. The mathematical background is formed by a series of papers by L.Faddeev, R.Minlos and F.Berezin [730, 731, 135] where point interactions are analysed in connection with the extension for symmetric operators in Hilbert spaces. In particular few-body problems with point interactions have been considered by these authors. It was observed that the spectral structure of the one-body problem with single point potential in $\mathbf{R}^3$ is simple (it includes, in particular, only one eigenvalue or one resonance). During the decade 1984–1994 a series of papers was published by St.Petersburg mathematicians (see [785, 786] for a review). In these papers a new sort of solvable model was introduced based on point interactions with internal structure. These models are related to the theory of generalized extensions of symmetric operators considered first by M.Krein. In fact Krein's formula relating the resolvents of arbitrary extensions of this type plays an important role in the investigation of such operators.

We will now describe the content of this monograph, at the same time taking the opportunity to make some complementary remarks. Let us stress that for historical remarks and background the basic reference we would like to give to the reader is [39] (which also indicates the original references).

In Chapter 1 rank one perturbations are studied. Thus we have a Hilbert space $\mathcal{H}$, a self–adjoint operator $\mathcal{A}$ and we study operators of the form $\mathcal{A}_\alpha = \mathcal{A}+\alpha\langle\varphi,\cdot\rangle\varphi$, with $\varphi \in \mathcal{H}$, $\langle\cdot,\cdot\rangle$ being the scalar product in $\mathcal{H}$, and $\alpha \in \mathbf{R}$. We look upon $\mathcal{A}_\alpha$ (and $\mathcal{A}$) as self–adjoint extensions of the symmetric operator $\mathcal{A}^0$ defined as $\mathcal{A}$ on

$$\mathrm{Dom}\,(\mathcal{A}^0) = \{\psi \in \mathrm{Dom}\,(\mathcal{A}) : \langle\varphi,\psi\rangle = 0\}.$$

The resolvent and spectral properties of $\mathcal{A}_\alpha$ are exhibited (using Krein's type of method). The case of "infinite coupling" corresponding to $\alpha = \infty$ is then shown to lead to a self–adjoint relation $\mathcal{A}_\infty$ instead of a self–adjoint operator. The case where φ does not belong to $\mathcal{H}$, but is still a linear bounded functional on Dom $(\mathcal{A})$ is analyzed in Section 1.2. Such finite rank perturbations are called "singular". In particular the cases of δ and δ'-perturbations of $-\frac{d^2}{dx^2}$ in $L_2(\mathbf{R}, dx)$ are considered (recovering results discussed in [39] from another point of view); we also recall that singular rank one perturbations were first studied in a rigorous mathematical sense by F.A.Berezin and L.D.Faddeev [135]. For the study of singular rank one perturbations it is useful to introduce a scale $\mathcal{H}_k(\mathcal{A}), k \in \mathbf{Z}$, of Hilbert spaces associated with $\mathcal{A}$. The vectors φ defining such perturbations belong to $\mathcal{H}_{-2}(\mathcal{A})$. We compare perturbations given by $\varphi \in \mathcal{H}_{-1}(\mathcal{A})$ and those given by $\varphi \in \mathcal{H}_{-2}(\mathcal{A})$. Moreover we relate the case $\varphi \in \mathcal{H}_{-2}(\mathcal{A})$ to the Krein–Krasnosel'skiĭ theory of self–adjoint extensions ($\mathcal{A}^0$ having deficiency indices $(1,1)$). In Section 1.3 we characterize the domain of self–adjoint extensions in the case of singular rank one perturbations, first in the "form bounded case" and then in the "form unbounded case". We also study the effect of perturbations in the situation where the original operator $\mathcal{A}$ and the element φ giving the perturbation are homogeneous with respect to a certain group of unitary transformations of the Hilbert space $\mathcal{H}$. We close the section by studying the resolvent of the perturbed operators. In Section 1.4 approximations of singular rank one perturbations by bounded rank one perturbations are discussed, first in the norm sense and then in the strong resolvent sense.

In Section 1.5 the results of the preceding sections are applied to the case of rank one perturbations of differential operators. We start out with a discussion of the basic model of a point interaction, i.e. an operator of the form $L_\alpha = -\Delta + \alpha\delta$, where Δ is the Laplacian acting in $L^2(\mathbf{R}^3)$ and $\alpha \in \mathbf{R}$. In their original work in 1961 F.A.Berezin and L.D.Faddeev [135] already pointed out the necessity of "renormalizing" the coupling constant α to get a non–trivial self–adjoint realization of L_α. In fact they described the self–adjoint realizations of L_α via Krein's theory of self–adjoint extensions of $-\Delta|C_0^\infty(\mathbf{R}^3 \setminus \{0\})$. Other descriptions of the family L_α have been given later on in terms of boundary conditions, as operators associated with Dirichlet forms [58, 59] and in terms of non–standard analysis [26, 79, 771] (in the latter description α appears to be given by $\epsilon + \tilde{\alpha}\epsilon^2$, where ϵ is an infinitesimal and $\tilde{\alpha}$ is the "renormalized coupling constant", belonging to $\mathbf{R}$ or equal to a certain positive infinite number). See also the books [39, 29]. In our treatment of L_α in the present book we look upon L_α as a singular rank one perturbation of $-\Delta$, given by the element $\delta \in \mathcal{H}_{-2}(-\Delta) \setminus \mathcal{H}_{-1}(-\Delta)$. By applying the results from the preceding section we exhibit in this way the domain of L_α, recover the expression for its resolvent and discuss the homogeneous character of the perturbation. We also discuss the boundary conditions satisfied at the origin by elements in the domain of L_α. Finally we introduce a space of generalized functions suitable to describe L_α. Moreover we relate the description of L_α with that of singularly perturbed Schrödinger operators on $L^2(0,\infty)$. We also apply the previous approximation results to the case of the operator L_α, exhibiting norm convergent approximations by $-\Delta$ perturbed by regular rank one perturbations. Strong resolvent convergence can be obtained by following the idea of renormalizing the coupling constant α. This has been described in [39]. In the present book we present another approach, based on [135], which uses Fourier transforms of distributions. We close the chapter by analyzing two problems of the theory of perturbations of first order operators. First we study operators of the form $A_\alpha = (1/i)\,(d/dx) + \alpha\delta$ on $L^2(\mathbf{R})$, then one dimensional Dirac operators with a delta potential.

In Chapter 2 we study generalized rank one perturbations of symmetric operators $\mathcal{A}^0$ in a Hilbert space $\mathcal{H}$. These perturbations are defined as extensions $\mathbf{A}$ of $\mathcal{A}^0$ such that $\mathbf{A}$ is a self–adjoint operator in an extended Hilbert space $\mathbf{H} \supset \mathcal{H}$. Thus whereas in Chapter 1 only extensions were studied with $\mathbf{H} = \mathcal{H}$ (so-called "standard" extensions), in Chapter 2 the case $\mathbf{H} \supset \mathcal{H}, \mathbf{H} \neq \mathcal{H}$, is studied. Krein's formula for the restriction to $\mathcal{H}$ of the resolvent of $\mathbf{A}$ ("generalized" resolvent) is derived and used to establish spectral properties. An explicit construction of generalized rank one perturbation is given in Section 2.2. Under a certain assumption this leads in particular to the interesting class of "operators with internal structure". The class of extensions of this type, given by operators with internal structure, is determined in terms of their resolvents, which are calculated explicitly. We first study the case of extensions of $\mathbf{A} = \mathcal{A} \oplus \mathcal{A}'$ characterized by two vectors, $\varphi \in \mathcal{H}_{-2}(\mathcal{A}) \setminus \mathcal{H}$ and $\varphi' \in \mathcal{H}_{-2}(\mathcal{A}') \setminus \mathcal{H}'$, where $\mathcal{H}' = \mathbf{H} \ominus \mathcal{H}$. We then study (Section 2.2.3) the case where $\varphi \in \mathcal{H}'$, where von Neumann's extension theory has to be replaced by the Krasnoselskiĭ extension theory. A characterization of generalized resolvents in terms of generalized perturbations with internal structure is also given (in Section 2.2.4). Applications of this theory to perturbations of differential operators are given in Section 2.3. We consider in particular in this setting the perturbations of $-\Delta$ by generalized point interactions described originally by B.Pavlov in terms of internal structure. We exhibit in particular their spectral properties and the resolvent, and determine their spectral quantities (eigenvalues, eigenfunctions, scattering amplitudes). We also study in detail the special case of the Hamiltonian for two one dimensional particles with a generalized delta interaction in one dimension. The self–adjoint extensions can be characterized in terms of "energy dependent" boundary conditions. We discuss in detail the scattering theory for such interactions. The operators studied in this chapter will also be of importance in Chapter 7 in order to construct the Hamiltonian describing a system of three one dimensional quantum particles with a δ-interaction.

In Chapter 3 singular perturbations of finite rank of self–adjoint operators are investigated, extending the results of Chapter 1 (which was devoted to rank one perturbations). Thus we consider operators of the form $\mathcal{A}_T = \mathcal{A}+T$, where $\mathcal{A}$ is a given self–adjoint operator in a Hilbert space $\mathcal{H}$ and T is a finite dimensional symmetric operator acting from $\mathcal{H}_2(\mathcal{A})$ to $\mathcal{H}_{-2}(\mathcal{A})$ (using the scale of Hilbert spaces mentioned above). We first study the case of a form bounded T. We start by exhibiting $\mathcal{A}_T$ as the self–adjoint restriction of the adjoint $\mathcal{A}^{0*}$ of a certain operator $\mathcal{A}^0$ which is the restriction of the operator $\mathcal{A}$ to a certain explicitly presented domain. Then we consider all self–adjoint extensions of $\mathcal{A}^0$. This theory will be latter applied to point interactions. Form unbounded finite rank perturbations are discussed in Section 3.1.3. We exhibit in particular their resolvent. The results are then extended to "generalized finite rank perturbations with internal structure" in the following subsection. Point interactions as finite rank perturbations of an n-order differential operator on the real line are studied in Section 3.2. Self–adjoint extensions are characterized in terms of "Lagrangian planes" of a boundary form. We develop a distribution theory for discontinuous test functions suitable for the description of the domains of the self–adjoint extensions. In Section 3.2.4 we look at the special case of second order differential operators providing a detailed description of all self–adjoint extensions in terms of explicit boundary conditions. Particular attention is dedicated to homogeneous properties of the extensions. All previous known results on interactions "located at a point" are recovered and extended. In particular δ and δ' interactions are described in a unified way.

In Chapter 4 the scattering theory for finite rank perturbations of self–adjoint operators is developed. The chapter starts out by discussing self–adjoint extensions of symmetric operators with finite deficiency indices. It is shown in particular that finite rank $\mathcal{H}_{-2}$-perturbations of self–adjoint operators leave the absolutely continuous spectrum invariant and any two operators which are self–adjoint extensions of a given symmetric operator with deficiency indices $(1,1)$ have unitary equivalent absolutely continuous parts. It is then shown that a generalized perturbation with internal structure of a self–adjoint operator has an absolutely continuous part equivalent to the latter if the extension space has finite dimension (Theorem 4.1.3). This is then extended to the equality of the continuous parts of any two self–adjoint extensions of a symmetric operator with finite deficiency indices (Theorem 4.1.4). The wave operators for rank one perturbations given by elements of $\mathcal{H}_{-1}(A)$ of a given self–adjoint operator A are computed (Theorem 4.1.5). In Section 4.2 the scattering theory (wave operators, scattering operator) for the case of two different self–adjoint extensions of a given symmetric operator with finite deficiency indices is worked out and applied to the cases of singular and generalized finite rank perturbations. Explicit formulae are given, e.g. in Theorem 4.2.1 and in Section 4.2.3. The special cases of finite rank perturbations is handled in Sections 4.3.1 and 4.3.2 whereas that of generalized perturbations is treated in Section 4.3.3.

In Chapter 5 a generalization of Krein's formula relating the resolvent of two self–adjoint extensions of a given symmetric operator to the case where the deficiency indices are infinite is derived. In Section 5.1.1 a description is given of the adjoint operator $\mathcal{A}^{0*}$ of the restriction of a self–adjoint operator $\mathcal{A}$ to a densely defined symmetric closed operator $\mathcal{A}^0$. An extension $\mathcal{A}^\Gamma$ of $\mathcal{A}^0$ determined by a self–adjoint "boundary" operator Γ in the deficiency subspace is studied. Applications to generalized perturbations of infinite rank are given in Section 5.1.2. A class of decomposable boundary operators is introduced and associated self–adjoint operators are studied. In Section 5.2 the results are specialized to the study of two-body quantum mechanical problems with interaction of rank one. The discussion is based on the concepts of Nevanlinna functions and the Stieltjes transform, which are summarized in Section 5.2.1. The resolvent of the operator $\mathcal{A}^\Gamma$ is computed using the fact that the operator $\mathcal{A}^\Gamma$ is a restriction of the adjoint operator $\mathcal{A}^{0*}$. The case of $\mathcal{H}_{-1}$ perturbations is given special attention. In Section 5.2.2 the considerations are extended to the study of two-body quantum mechanical operators with generalized interactions of rank one, with applications to quantum mechanical models with internal structure (Theorems 5.2.3 and 5.2.4).

In Chapter 6 a Krein type formula is derived for the study of few-body quantum mechanical problems. Operators describing few-body problems with "cluster interactions" of rank one are introduced and studied. In Section 6.1.2 the case of $\mathcal{H}_{-1}$-interactions is studied in detail, whereas in Section 6.1.3 the case of $\mathcal{H}_{-2}$-interactions is investigated. The concept of separable, respectively, strongly separable interactions is introduced. The separable case is handled in Section 6.1.3. In the strongly separable case $\mathcal{H}_{-2}$ as well as $\mathcal{H}_{-1}$ perturbations are handled, and the resolvent is computed (Theorem 6.1.5). The concepts of separable/non-separable are discussed in Section 6.1.5 for the important case of three particles moving in $\mathbf{R}^n$ with two–body and three–body interactions. In Section 6.2 the case of several quantum mechanical particles with generalized interactions is discussed. It is proven that the corresponding few–body operator is selfadjoint and bounded from below even if the interactions are infinitesimally separable (not necessarily strongly separable as for usual singular interactions).

In Chapter 7 we discuss models describing the motion of three quantum mechanical particles interacting through multiparticle forces in one dimension. In Section 7.1 we study the system consisting of three one-dimensional particles with two-particle interactions of the "δ-function" type (point interactions). For simplicity we assume all masses to be equal. A first step (Sections 7.1.1 and 7.1.2) consists in defining the one-parameter family of Schrödinger operators (Hamiltonians) for this system. The construction is achieved following the method described in the preceding chapter. In Section 7.1.3 we study the spectrum and eigenfunctions of the constructed operators. The eigenfunctions are exactly described by the Bethe Ansatz iff all coupling constants α_γ describing the two-body interactions are equal. In this case we exhibit the eigenfunctions explicitly. In Section 7.2 we extend our study to the case of three quantum mechanical particles with generalized two-body delta interactions (as discussed in Chapter 2, Section 2.2). In Sections 7.2.1 and 7.2.2 the corresponding Hamiltonians are constructed. To discuss the corresponding eigenfunctions we restrict ourselves first to the case where all particles are bosons, respectively, fermions. The necessary consideration of Bose, respectively, Fermi symmetry are given in Section 7.2.3. The outgoing wave appearing in the study of eigenfunctions for such a system of bosons is discussed in detail in Section 7.2.4, following [635] (which in turn used analytic methods introduced by Sommerfeld and Malyuzhinets in optics). The calculation of the outgoing wave is reduced essentially to the solution of a system of functional equations, discussed in Section 7.2.5, using methods of classical complex analysis of meromorphic functions. Detailed analytic properties of the solution are exhibit in Theorem 7.2.2. To find the outgoing waves themselves a study of the asymptotics in a space parameter is undertaken in Section 7.2.6. The spectrum and the scattering matrix for the Hamiltonians are derived in Section 7.2.7. The final result for the scattering matrix, after detailed calculations, is expressed in terms of elementary functions. The case of non–identical particles is also briefly discussed.

Appendix A contains historical remarks concerning basic references used in the text and developments after the publication of [39, 40], whereas we refer basically to [39, 40] for previous references.

We would like to mention that we see the role of solvable models constructed by methods of extension theory in mathematical and theoretical physics as complementary to the role played by quasiclassical analysis (respectively geometrical optics in electromagnetic theory). The latter is aimed at handling problems where the typical size of perturbation is greater than the typical wavelength of the process. Vice versa, point interactions and generalized point interactions are appropriate approximations in problems where the typical wavelength of the process is greater than the size of the perturbation. The quasiclassical approximation usually gives explicit formulas for solutions of partial differential operators (wave functions in quantum mechanical problems), but the calculation of the corresponding spectral characteristics needs additional effort and assumptions. In solvable models with point interactions we usually have to deal with a self–adjoint operator which approximates the original Hamiltonian. Then all spectral characteristics of this operator are calculated in explicit form and serve as approximations for the corresponding spectral characteristics of the original problem. This opens the way to spectral modeling, that is producing models which possess relevant spectral properties. In particular, we may fit some spectral properties into a two-body Hamiltonian with a generalized point interaction and then calculate the spectral properties of the corresponding few-body model.

Thus the use of solvable models is natural and useful in numerous problems of few-body scattering, nanoelectronics, the theory of neural networks, as well as in acoustics, hydrodynamics and elasticity – each time, when the typical wavelength is greater than the size of the perturbation. We hope that the methods described in the present book will find further numerous applications in the study of such problems.

Cambridge University Press
978-0-521-77912-8 - Singular Perturbations of Differential Operators: Solvable Schrodinger Type Operators
S. Albeverio and P. Kurasov
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Chapter 1

Rank one perturbations

1.1 Bounded perturbations

1.1.1 Resolvent analysis

Let us start our investigation of finite rank perturbations of self–adjoint operators with the simplest sort of perturbation – a rank one bounded perturbation. Let A be a self–adjoint (perhaps unbounded) operator in the Hilbert space H with domain Dom (A). Let φ be a vector from the Hilbert space, $\varphi \in H$ and α be a real number, $\alpha \in \mathbf{R}$. A symmetric rank one bounded perturbation of A is the operator defined by the following formula

$$A_\alpha = A + \alpha \langle \varphi, \cdot \rangle \varphi, \tag{1.1}$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product in the Hilbert space H. The rank one operator $\alpha \langle \varphi, \cdot \rangle \varphi$ is a bounded operator in the Hilbert space and the operator sum A_α is well defined. Actually the operator A_α is self–adjoint on the domain Dom (A) of the operator A. The spectral properties of the perturbed operator can be obtained using its resolvent, which can be calculated using Krein's formula connecting the resolvents of two self–adjoint extensions of one symmetric operator with finite deficiency indices (see Section 1.2.5). In fact the operators A_α and A are two self–adjoint extensions of the symmetric operator A^0 being the restriction of the operator A to the set of all functions orthogonal to the vector φ :

$$\mathrm{Dom}\,(A^0) = \{\psi \in \mathrm{Dom}\,(A) : \langle \varphi, \psi \rangle = 0\}.$$

The operator A^0 is a symmetric nondensely defined operator, since $\varphi \in H$. Self–adjoint extensions of such symmetric operators have been studied by M. A. Krasnosel'skiĭ [561, 562]. The resolvent of the operator A_α can be calculated in this case without using the extension theory for symmetric operators.

Theorem 1.1.1 *Let A be a self–adjoint operator acting in the Hilbert space H and let φ be arbitrary vector from the Hilbert space, $\varphi \in \mathcal{H}$. Then the resolvents of the original operator A and its rank one perturbation $A_\alpha = A + \alpha\langle\varphi,\cdot\rangle\varphi$, $\alpha \in \mathbf{R}$, are related as follows for arbitrary $z, \Im z \neq 0$,*

$$\frac{1}{A_\alpha - z} - \frac{1}{A-z} = -\frac{\alpha}{1+\alpha F(z)} \left\langle \frac{1}{A-\bar{z}}\varphi, \cdot \right\rangle \frac{1}{A-z}\varphi, \tag{1.2}$$

where

$$F(z) = \left\langle \varphi, \frac{1}{A-z}\varphi \right\rangle. \tag{1.3}$$

Proof To calculate the resolvent of the self–adjoint operator A_α we have to solve the following equation

$$h = (A_\alpha - z)f,$$

for a given $h \in H$ and $f \in \mathrm{Dom}\,(A_\alpha) = \mathrm{Dom}\,(A)$. We assume that the imaginary part of the spectral parameter z is positive $\Im z > 0$. We apply the operator $A_\alpha - z$ to the latter equality

$$\begin{aligned} h &= (A + \alpha\langle\varphi,\cdot\rangle\varphi - z)\, f \\ &= Af - zf + \alpha\langle\varphi, f\rangle\varphi. \end{aligned}$$

By applying the resolvent of the original operator we get

$$\frac{1}{A-z}h = f + \alpha\langle\varphi, f\rangle \frac{1}{A-z}\varphi.$$

Projection on the vector φ leads to the following formula for $\langle\varphi, f\rangle$

$$\langle\varphi, f\rangle = \frac{\langle\varphi, \frac{1}{A-z}h\rangle}{1+\alpha\langle\varphi, \frac{1}{A-z}\varphi\rangle}.$$

It follows that

$$f = \frac{1}{A-z}h - \frac{\alpha}{1+\alpha\langle\varphi, \frac{1}{A-z}\varphi\rangle}\left\langle \varphi, \frac{1}{A-z}g \right\rangle \frac{1}{A-z}\varphi,$$

which is exactly formula (1.2). The theorem is proven.

□