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Self-adjointness of Quantum Hamiltonians with Symmetries

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Abstract

This thesis discusses the general problem of the self-adjoint realisation of formal Hamiltonians with a focus on a number of quantum mechanical models of actual relevance in the current literature, which display certain symmetries. In the first part we analyse the general extension theory of (possibly unbounded) linear operators on Hilbert space, and in particular we revisit the Kreĭn-Višik-Birman theory that we are going to use in the applications. We also discuss the interplay between extension theory and presence of discrete symmetries, which is the framework of the present work.

The second part of the thesis contains the study of three explicit quantum models, two that are well-known since long and a more modern one, each of which is receiving a considerable amount of attention in the recent literature as far as the identification and the classification of the extensions is concerned. First we characterise all self-adjoint extensions of the Hydrogen Hamiltonian with point-like interaction in the origin and of the Dirac-Coulomb operators. For these two operators we also provide an explicit formula for the eigenvalues of every self-adjoint extension and a characterisation of the domain of respective operators in term of standard functional spaces. Then we investigate the problem of geometric quantum confinement for a particle constrained on a Grushin-type plane: this yields the analysis of the essential self-adjointness for the Laplace-Beltrami operator on a family of Riemannian manifolds.

Contents

Introduction

To the present understanding of Nature, microscopic world is ruled by quantum mechanics. In its axiomatic definition, states are element of a Hilbert space $\mathcal{H}$ and observables are self-adjoint operators on $\mathcal{H}$. Deep physical reasons, such as Heisenberg's uncertainty principle, let alone the very mathematical modelling of the quantum system, in many relevant cases make it unavoidable for the observables to be represented as (densely defined) unbounded self-adjoint operators on $\mathcal{H}$. This gives rise to a primary conceptual problem – the rigorous self-adjoint realisation of physical Hamiltonians – that in a vast generality is surely under control since Kato's proof of self-adjointness of molecular Hamiltonians in the 1950's, and yet turns out to be most topical in many instances of today's research agenda, when new quantum systems of physical interest are investigated, or well-studied quantum Hamiltonians are revisited with more modern and more general mathematical tools.

This thesis is part of the above-outlined research programme and discusses the realisation of some formal physical Hamiltonians as self-adjoint operators. In particular, motivated by their importance in physics, we are concerned with Hamiltonians that are invariant under the action of symmetry groups.

Let us present, in simple words, where the theory of self-adjoint realisations enters in quantum mechanics. When we are describing a quantum mechanical system on a Hilbert space $\mathcal{H}$, a physical procedure (usually first quantisation) provides a formal expression for an observable T on $\mathcal{H}$.

If T is a pseudodifferential expression (as is often the case), two standard choices for the domain are avaible: the minimal and the maximal one (Section 1.2). In assigning these domains, we construct two (a priori) different operators, $T_{\min}$ and $T_{\max}$, as realisations of the same formal expression T. Under some hypothesis on the minimal operator that are often met in realistic problems, such as the presence of a spectral gap or the existence of a bottom, von Neumann's celebrated theorem (Theorem 1.3.1) guarantees the existence of at least one self-adjoint extension of the minimal operator, and shows that such extension lies between $T_{\min}$ and $T_{\max}$ (in the operator inclusion sense). In fact, only two possibilities are allowed: either there is only one self-adjoint realisation of T on $\mathcal{H}$ or there are infinitely many. In the first case, the association of an observable to the formal expression T is unambiguous since, in this case, the minimal and the maximal operator coincide. The second case is more challenging and one major issue is to classify all self-adjoint extensions of $T_{\min}$ in order to construct all quantum observables associated with the formal expression T. At this point a *self-adjoint extension theory* is needed (a la von Neumann or a la Kreĭn-Višik-Birman).

When T is invariant under some simmetry group, one may decompose the Hilbert space into orthogonal subspaces that reduce T, thus simplifying the analysis of T boiling it down to the analysis of each component of T. At this point it may happen that some of the extensions of the minimal operator are not invariant under the action of the symmetry group. It is therefore physically relevant to determine which ones preserve the symmetry and which ones do not.

Self-adjoint extension theory

Self-adjointness and self-adjoint extension theory constitute a well-established branch of functional analysis and operator theory, with deep-rooted motivations and applications, among others, in the boundary value problems for partial differential equations and in the mathematical methods for quantum mechanics and quantum field theory. As recalled in the previous section, at the highest level of generality, it is von Neumann's celebrated theory of self-adjoint extensions that provides, very elegantly, the complete solution to the problem of finding self-adjoint operator(s) that extend a given densely defined symmetric operator S on a given Hilbert space $\mathcal{H}$. As well known, the whole family of such extensions is naturally indexed by all the unitary maps U between the subspaces $\ker(S^* - z)$ and $\ker(S^* - \overline{z})$ of $\mathcal{H}$ for a fixed $z \in \mathbb{C} \setminus \mathbb{R}$, the condition that such subspaces be isomorphic being necessary and sufficient for the problem to have a solution; each extension S_U is determined by an explicit constructive recipe, given U and the above subspaces.

A relevant special case is when S is semi-bounded – one customarily assumes it to be bounded *below*, and so shall we henceforth – which is in fact a typical situation in the quest for stable quantum mechanical Hamiltonians. In this case $\ker(S^* - z)$ and $\ker(S^* - \overline{z})$ are necessarily isomorphic, which guarantees the existence of self-adjoint extensions. Among them, a canonical form construction (independent of von Neumann's theory) shows that there exists a distinguished one, the Friedrichs extension S_F, whose bottom coincides with the one of S, which is characterised by being the only self-adjoint extension whose domain is entirely contained in the form domain of S, and which has the property to be the largest among all self-adjoint extensions of S, in the sense of the operator ordering "$\geqslant$" for self-adjoint operators.

By the Kreĭn-Višik-Birman (KVB) theory (where the order here reflects the chronological appearance of the seminal works of Kreĭn [74], Višik [112], and Birman [15]), one means a development of Kreĭn's original theory, in the form of an *explicit* and *extremely convenient* classification of all self-adjoint extensions of a given semi-bounded and densely defined symmetric operator S, both in the operator sense and in the quadratic form sense.

The KVB theory has a number of features that make it in many respects more informative as compared to von Neumann's. First and most importantly, the KVB parametrisation $B \leftrightarrow S_B$ identifies special subclasses of extensions of S, such as those whose bottom is above a prescribed level, in terms of a corresponding subclass of parameters B. In particular, both the Friedrichs extension S_F and the Kreĭn-von Neumann extension S_N of S relative to a given reference lower bound can be selected a priori, meaning that the special parameter B that identifies S_F or S_N is explicitly known. In contrast, the parametrisation $U \leftrightarrow S_U$ based on unitaries U provided by von Neumann's theory does not identify a priori the particular U that gives S_F or S_N. An amount of further relevant information concerning each extension, including invertibility, semi-boundedness, and special features of its negative spectrum (finiteness, multiplicity, accumulation points) turn out to be controlled by the the analogous properties of the extension parameter. Furthermore, the KVB extension theory has a natural and explicit re-formulation in terms of quadratic forms, an obviously missing feature in von Neumann's theory. On this last point, it is worth emphasizing that whereas the KVB classification of the extensions as *operators* is completely general, the classification in terms of the corresponding *quadratic forms* only applies to to the family of *semi-bounded* self-adjoint extensions of S, while unbounded below extensions (if any) escape this part of the theory.[1]

For several historical and scientific reasons (a fact that itself would indeed deserve a separate study) the mathematical literature in English language on the KVB theory is considerably more

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[1]If the subspaces $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \overline{z}\mathbb{1})$ have the same *finite* dimension, it is easy to conclude that all self-adjoint extensions of S are bounded below, see, e.g., the Proposition on page 179 of [95]; if their common dimension is *infinite* instead, S may also admit self-adjoint extensions that are unbounded below. The occurrence of such unbounded below extensions may be presented as a mere "academic exercise" about operators on an infinite orthogonal sum of Hilbert spaces (see [95, Chapter 10], Problem 26) but in fact examples are known where they arise as quantum Hamiltonians of physical relevance – see, e.g., the possibility of unbounded below self-adjoint extensions for particle Hamiltonians with point interaction [88, 87, 82, 83, 31, 84].

limited as compared to von Neumann's theory. Over the decades the tendency has been in general to re-derive and discuss the main results through routes and with notation and "mathematical flavour" that differ from the original formulation.

At the price of an unavoidable oversimplification, we can say that while in the applications to quantum mechanics von Neumann's theory has achieved a dominant role, and is nowadays a textbooks standard, on a more abstract mathematical level the original results of Kreĭn, Višik, and Birman, and their applications to boundary value problems for elliptic PDE, have eventually found a natural evolution and generalisation within the modern theory of boundary triplets. Thus, in modern terms the deficiency space $\ker(S^* + \lambda\mathbb{1})$ is referred to as a *boundary value space*, this space is then equipped with a *boundary triplet structure*, and the extensions of S are parametrised by *linear relations* on the boundary space, with a distinguished position for the Friedrichs and the Kreĭn-von Neumann extensions that are intrinsically encoded in the choice of the boundary triplet.

However, our work [51] and Chapter 2 are *neither* meant *nor* going to move from the point of view of the boundary triplet theory, which is surely a beautiful and prolific scheme within which one can indeed retrieve the old results of Kreĭn, Višik, and Birman – in fact, the latter approach is already available in the literature: for example a recent, concise, and relatively complete survey of the re-derivation of Kreĭn, Višik, and Birman from the boundary triplet theory may be found in [104, Chapters 13 and 14], and in the references therein.

Symmetries of self-adjoint operators

We have already commented on the possibility that the formal T experiences a given symmetry and yet some if its extensions do not.

In the models discussed in this thesis we consider specifically *compact* symmetry groups. In practice the Hilbert space of interest is decomposed into an orthogonal sum of L^2-spaces over the (half-)line. In this setting, the reduced operator is an ordinary differential operator, which is simpler to study than a partial differential operator. In Chapter 3, we present general results concerning how to re-assemble all the information on the reduced operators in order to construct a self-adjoint realisation of the initial operator.

Applications

The tools described in the previous sections are used in the second part of the thesis to classify all self-adjoint realisations of the formal Hamiltonians for three physical problems: Hydrogen atom with point interaction at the origin, Dirac operator with Coulomb interaction in the critical regime of the coupling constant, and the Laplace-Beltrami operator on Grushin-like manifolds. These problems are solved using the following strategy, which is also the structure of my works [50, 52, 49]:

- the presence of a symmetry that allows one to reduce the analysis to ordinary differential operators on the half-line;

- first, reduced operators are analysed by means of Weyl's limit-point/limit-circle criterion of essential self-adjointness (see Section 1.4);

- the kernel of the adjoint of the reduced one-dimensional ordinary differential operator is known in terms of special functions, specifically confluent hypergeometric, Whittaker and modified Bessel functions;

- the inverse of a distinguished extension can be written explicitly using Green function methods;

- further, one estimates the behaviour close to the origin of functions in the domain of the minimal realisation of the reduced ordinary differential operator;

- at this point all ingredients to apply KVB theory are known, which allows one to identify the domains of all self-adjoint realisations by suitable boundary conditions at the origin connecting the 'regular part' to the 'singular part' of every function in the domain of the maximal realisation of the ordinary differential operator.

Hydrogen Hamiltonians with point-like perturbation at the centre

As a first example of quantum mechanical Hamiltonian with symmetry, we are concerned with certain realistic types of perturbations of the familiar quantum Hamiltonian for the valence electron of hydrogenoid atoms, namely the formal operator

$$H_{\text{Hydr}} \;=\; -\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{|x|} \tag{$\star$}$$

on $L^2(\mathbb{R}^3)$, where m and $-e$ are, respectively, the electron's mass and charge ($e > 0$), Z is the atomic number of the nucleus, $\hbar$ is Planck's constant and Δ is the three-dimensional Laplacian.

Intimately related to the three dimensional problem ($\star$), we are concerned with its radial counterpart

$$h_0^{(\nu)} \;=\; -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\nu}{r} \tag{$\star\star$}$$

with $\nu = -Ze^2$ in units where $2m = \hbar = 1$. Indeed, as we shall discuss more precisely in Chapter 4, spherical symmetry reduces the problem of self-adjoint realisation of the three dimensional operator ($\star$) into the problem of self-adjoint realisation of ($\star\star$). This radial problem is already discussed in Schrödinger's paper [105] to find energy levels of the Hydrogen atom. The model with delta interaction in the origin is known as *Darwin Hamiltonian* and it was introduced by Darwin [33] as a relativistic correction of the Hydrogen Hamiltonian ($\star$) in the *s*-wave sector.

From a mathematical perspective, the first analysis dates back to to Rellich [98] (even though self-adjointness was not the driving notion back then) and is based on Green's function methods to show that $-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\nu}{r} + \mathrm{i}\mathbb{1}$ is inverted by a bounded operator on Hilbert space when the appropriate boundary condition at the origin is selected. Some four decades later Bulla and Gesztesy [21] (a concise summary of which may be found in [4, Appendix D]) produced a 'modern' classification based on the special version of von Neumann's extension theory for second order differential operators [118, Chapter 8], in which the extension parameter that labels each self-adjoint realisation governs a boundary condition at zero. More recently Gesztesy and Zinchenko [54] extended the scope of [21] to more singular potentials than r^{-1}. Dereziński and Richard [35] instead studied several properties of the Whittaker operator (which is a generalisation of ($\star\star$) where ν is allowed to be a complex number and one adds a complex-valued centrifugal term) with the main goal of establishing which properties are preserved when all parameters are allowed to be complex (and hence, the operator is not anymore self-adjoint).

The novelty of the analysis in my work [49], in collaboration with A. Michelangeli, consists in the explicit qualification of the closure and of the Friedrichs extension of $h_0^{(\nu)}$, and in the classification of all self-adjoint extensions for ($\star$)-($\star\star$) obtained through the relatively straightforward application of the extension scheme of Kreĭn, Višik, and Birman (as an alternative path with respect to the above-mentioned works).

On the physical side of the physical literature on the subject, the one dimensional model has attained a certain amount of attention since [43] (and for a recent review we refer to [81]). On one side, many different approaches have been proposed to find eigenvalues and eigenfunctions of the problem, on the other side it has been looked for some experimental realisation of a system described by ($\star\star$). This problem is still under active investigation, as it may be seen some recent publications, e.g. [23].

Dirac-Coulomb operator in the critical regime

The Dirac-Coulomb system is a model for a relativistic electron subjected to the electrostatic attraction of a positively-charged nucleus placed at the origin. The formal expression of the Hamiltonian is

$$H \;=\; -\mathrm{i}\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta + \frac{\nu}{|x|}\mathbb{1}$$

as an operator acting on $L^2(\mathbb{R}^3, \mathbb{C}^4)$. Here $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and $\alpha_1, \alpha_2, \alpha_3, \beta$ are 4×4 Hermitian and anticommuting matrices (see e.g. (5.1.3)) and $\nu \in \mathbb{R}$ is the nucleus charge. The problem of the self-adjointness of H has a long story that dates back to Rellich [98] and Kato [69] who established its self-adjointness for $|\nu| < \frac{1}{2}$ by means of perturbative arguments. Adapting the perturbative argument several authors proved the essential self-adjointness of the operator reaching the optimal value of $\nu = \frac{\sqrt{3}}{2}$ [97, 61, 103, 28, 42, 77, 117].

Many subsequent works [102, 89, 123, 41, 11] aimed at constructing a physically distinguished self-adjoint realisation of the model. It was proved that if $|\nu| < 1$, there is only one self-adjoint extension whose the domain is contained in $H^{1/2} \cap \mathcal{D}(r^{-1/2})$. Physically this requirement amounts to having finite expectation of both kinetic and potential energy. In the literature it is custumary to refer to this particular self-adjoint realisation as the *distinguished* extension. In the work [47] I reviewed the history of the problem and the main ideas of the proofs.

We can distinguish among three regimes:

- the *subcritical* regime $|\nu| \leqslant \frac{\sqrt{3}}{2}$, where the minimal operator is essentially self-adjoint;

- the *critical* regime $\frac{\sqrt{3}}{2} < |\nu| < 1$, where the radial operator has a one real parameter family of self-adjoint realisations and there exists a distinguished one in the sense above mentioned.

- the *overcritical regime*, where the deficency indices depend on $|\nu|$ and no distinguished extension exists.

Only a few works in the existing literature on Dirac-Coulomb operators were concerned with the classification of its self-adjoint extensions [114, 64] and both were based upon von Neumann's theory.

In work [50], together with A. Michelangeli, I applied the KVB theory instead, in order to classify all the self-adjoint realisations of the radial Dirac-Coulomb operator in the critical regime. As it is well-known, Dirac-Coulomb operators are not semi-bounded but thanks to the presence of a spectral gap we could apply Grubb's version of KVB theory [60, Section 13] to classify the extensions. Working out resolvent formulas we could additionally produce a reliable estimate of the ground state of each extension.

All extensions turn out to have the same absolutely continuous spectrum, owing to Kuroda-Birman Theorem [104, Theorem 9.29 (ii)], since their resolvents differ by a rank-one operator from the resolvent of the distinguished extension.

As for the discrete spectra of the extensions, we classified them in my work [48]. In particular, we solved explicitly the eigenvalue equation for the generic self-adjoint extension of the model and we explained how the two classical ways to compute eigenvalues, by means of supersymmetric methods [111, Section 5.5.2] (or the works [30, 57, 91, 109]) or truncation of series (see e.g. [14, Section 16]), select naturally two self-adjoint realisations only: the distinguished one and another one which we named the 'mirror-distinguished'.

Geometric Quantum confinement in Grushin-type manifolds

When a quantum particle is constrained on an orientable Riemannian manifold M, one challenging problem that arises naturally is the question of the so-called *geometric quantum confinement*. The Hilbert space of the system is $L^2(M, \mathrm{d}\mu_g)$, where μ_g is the volume form induced by the Riemannian

metric on M, and the Schrödinger Hamiltonian of interest is a self-adjoint realisation of the operator $H = -\Delta_\mu + V$ where $-\Delta_\mu$ is the Laplace-Beltrami operator computed with respect to the measure μ and V is a real-valued potential on M. Informally speaking, in this setting we have geometric quantum confinement when $-\Delta_\mu$ on $C_0^\infty(M)$ is essentially self-adjoint. Physically this means that the quantum particle does not reach the boundary of the manifold and hence it is confined by the geometry of the space and not by boundary conditions. In fact, boundary conditions encode an interaction of the boundary ∂M with the particle localised in M and if $C_0^\infty(M)$ is a domain of essential self-adjointness for H it is natural to interpret this as a confinement in M not due to the boundary (but to the sole geometry instead).

The case of smooth and geodesically complete Riemannian manifolds is relatively well-understood [46, 18]. For incomplete Riemannian manifolds the picture is less developed, yet fairly general classes of V's are known which ensure the self-adjointness of Schrödinger operators on bounded domains of $\mathbb{R}^d$ with smooth boundary of co-dimension 1 [90] or more generally on bounded domains of $\mathbb{R}^d$ with non-empty boundary [115].

Quantum confinement on manifolds equipped with the so-called *almost-Riemannian structure* has attracted considerable attention over the last years [16, 93, 44].

In the work [52], in collaboration with A. Michelangeli and E. Pozzoli, I studied this problem in a class of two-dimensional incomplete Riemannian manifolds with metric of Grushin type, i.e.,

$$g_\alpha = \mathrm{d}x \otimes \mathrm{d}x + \frac{1}{|x|^{2\alpha}} \mathrm{d}y \otimes \mathrm{d}y$$

with $(x, y) \in (\mathbb{R} \setminus \{0\}) \times \mathbb{R}$ and $\alpha \in [0, +\infty)$. Calling μ_g the volume form associated with the metric g_α, one can first simplify the problem by considering the splitting $L^2(\mathbb{R}^2, \mathrm{d}\mu_g) = L^2(\mathbb{R}^- \times \mathbb{R}, \mathrm{d}\mu_g) \oplus L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}\mu_g)$. The analysis of the essential self-adjointness boils down to the analysis of essential self-adjointness on each of the two reducing subspaces. Each of these subspaces can be written as constant-fibre direct integral as $L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}\mu_g) = \int_\mathbb{R}^\oplus L^2(\mathbb{R}^+, \mathrm{d}x)\, \mathrm{d}\xi$ (and an analogous formula for $L^2(\mathbb{R}^-, \mathrm{d}\mu_g)$). On each fibre we used Weyl's criterion to fully characterise the regimes of presence and absence of essential self-adjointness of the associated Laplace-Beltrami operator (i.e., the regimes of presence or absence of quantum confinement).

In the case of $\alpha \in [0, 1)$, the Laplace-Beltrami operator is not essentially self-adjoint and, with respect to the constant-fibre direct integral decomposition $L^2(\mathbb{R}^2, \mathrm{d}\mu_g) = \int_\mathbb{R}^\oplus \left(L^2(\mathbb{R}^-, \mathrm{d}x) \oplus (L^2(\mathbb{R}^+, \mathrm{d}x)\right)\mathrm{d}\xi$, the minimal operator on each fibre has deficiency indices $(2, 2)$. The problem of classification of all self-adjoint extensions of this operator is an interesting issue that will be addressed in the future.

Structure of the thesis

The material in the thesis is organised in two parts. In the first part we present the theory starting in Chapter 1 with basic definitions, von Neumann extension theory and Weyl's criterion. In Chapter 2 we present the content of my work [51], in collaboration with A. Michelangeli and A. Ottolini, where it is revisited the Kreĭn-Višik-Birman extension theory. In Chapter 3 we present a decomposition result for symmetric spaces and we present the relation of self-adjoint extension theory and the reduction by symmetry.

In the second part of the thesis we present some applications of the theory above. Chapter 4 presents the content of my work [49], in collaboration with A. Michelageli, which analyses the rigorous construction of the Hamiltonian of the Hydrogen atom plus a delta interaction placed in the origin within the framework of KVB theory. Chapter 5 presents my works [47, 50, 48] (in collaboration with A. Michelangeli) and it analyses the self-adjoint realisations of the Dirac-Coulomb operator in the *critical* regime of the coupling constant. Last application, in Chapter 6, presents my work [52] in collaboration with A. Michelangeli and E. Pozzoli.

Last, in the Appendix we present the proof of a decomposition result of symmetric spaces.

General Notation. Essentially all the notation adopted here is standard, let us only emphasize the following. Concerning the Hermitian scalar product we adopt the convention of being linear in the second entry. Concerning the various sums of spaces that will occur, we shall denote by $\dotplus$ the direct sum of vector spaces, by $\oplus$ the direct orthogonal sum of *closed* Hilbert subspaces of the same underlying Hilbert space $\mathcal{H}$ (the space where the initial symmetric and densely defined operator is taken), and by $\boxplus$ the direct sum of subspaces of $\mathcal{H}$ that are orthogonal to each other but are not a priori all closed. For any given symmetric operator S with domain $\mathcal{D}(S)$, we shall denote by $m(S)$ the "bottom" of S, i.e., its greatest lower bound

$$m(S) \ := \ \inf_{\substack{f \in \mathcal{D}(S) \\ f \neq 0}} \frac{\langle f, Sf \rangle}{\|f\|^2} \,.$$

S being semi-bounded means therefore $m(S) > -\infty$. Let us also adopt the customary convention to distinguish the *operator* domain and the *form* domain of any given densely defined and symmetric operator S by means of the notation $\mathcal{D}(S)$ vs $\mathcal{D}[S]$. To avoid ambiguities, $V^{\perp}$ will always denote the orthogonal complement of a subspace V of $\mathcal{H}$ *with respect to $\mathcal{H}$ itself*: when interested in the orthogonal complement of V within a closed subspace K of $\mathcal{H}$ we shall keep the extended notation $V^{\perp} \cap K$. Analogously, the closure $\overline{V}$ of the considered subspaces will be always meant with respect to the norm-topology of the underlying Hilbert space $\mathcal{H}$. As no particular ambiguity arises in our formulas when referring to the identity operator, we shall use the symbol $\mathbb{1}$ for it irrespectively of the subspace of $\mathcal{H}$ it acts on. As for the spectral measure of a self-adjoint operator A we shall use the standard notation $\mathrm{d}E^{(A)}$ (see, e.g., [104, Chapters 4 and 5]). As customary, $\sigma(T)$ and $\rho(T)$ shall denote, respectively, the spectrum and the resolvent set of an operator T on Hilbert space.

Apart from Appendix A, when the measure of L^p-spaces is not explicitly specified it is intended to be the Lebesgue measure.

Part I

General Theory

Chapter 1

Unbounded Differential Operators on Hilbert Spaces

The need of a theory of unbounded operators on Hilbert spaces was stimulated by attempts in the late 20s to put quantum mechanics on a rigorous mathematical framework. Indeed, from a purely physical point of view, Heisenberg uncertainty principle implies that at least one among position and momentum operator has to be unbounded. The systematic development of the theory is due to von Neumann [113] and Stone [108]. This subject is nowadays a classical part of functional analysis and we give in this chapter a concise summary that includes all the basic notions we are going to use in the following chapters. Since the material presented in this chapter is standard, we limit ourselves to quote references for details and proofs.

In the first Section we recall some standard definitions and in the second one we define two standard ways to realise a formal differential operator as an operator on the Hilbert space of square integrable functions. In Section 1.3 we present von Neumann's and Kreĭn's extension theory as well as some properties of some 'distinguished' self-adjoint realisations of a densely defined semi-bounded symmetric operator, namely the Friedrichs and the Kreĭn-von Neumann extensions. In Section 1.4 we present Weyl's alternative, a standard way to compute deficiency indices for symmetric ordinary differential operators.

1.1 Basic definitions

Definition 1.1.1. A *linear operator* from a Hilbert space $\mathcal{H}$ into itself is a linear map T from a linear subspace $\mathcal{D}(T) \subset \mathcal{H}$ (called the *domain* of T) into $\mathcal{H}$.

Together with the domain, one defines also the *range*

$$\operatorname{ran} T \; := \; \{T\psi \,|\, \psi \in \mathcal{D}(T)\} \tag{1.1.1}$$

and the *kernel* of T

$$\ker T \; := \; \{\psi \in \mathcal{D}(T) \,|\, T\psi = 0\}\,. \tag{1.1.2}$$

By a *restriction* of an operator T on a subset $\mathcal{D} \subset \mathcal{D}(T)$ we mean the operator $S : \mathcal{D} \to \mathcal{H}$ such that $S\psi = T\psi$ for all $\psi \in \mathcal{D}$. To denote that S is a restriction of T we write $S \subset T$. We say that T is an *extension* of S if S is a restriction of T.

The *graph* of a linear operator T is the subspace $\Gamma(T) \subset \mathcal{H} \oplus \mathcal{H}$, defined as

$$\Gamma(T) \; := \; \{(\psi, T\psi) \,|\, \psi \in \mathcal{D}(T)\}\,. \tag{1.1.3}$$

Definition 1.1.2. A linear operator T on $\mathcal{H}$ is *closed* if $\Gamma(T)$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$.

An operator is said to be *closable* if there exists a closed operator S such that $T \subset S$. If a linear operator T is closable, the closure of its graph defines the graph of another operator called the *closure* of T and denoted by $\overline{T}$:

$$\Gamma(\overline{T}) \ = \overline{\Gamma(T)} \,. \tag{1.1.4}$$

Alternatively one sees that on $\mathcal{D}(T)$ we can define a norm, called *operator norm* (or sometimes also *graph norm*) which is

$$\|\psi\|_T^2 \ := \ \|T\psi\|_{\mathcal{H}}^2 + \|\psi\|_{\mathcal{H}}^2 \qquad \text{for } \psi \in \mathcal{D}(T) \,. \tag{1.1.5}$$

A set $\mathcal{D} \subset \mathcal{D}(T)$ is a *core* for T if $\mathcal{D}$ is dense in $\mathcal{D}(T)$ in the topology induced by the operator norm.

Definition 1.1.3. Given a linear operator T, its adjoint is the linear operator T^* defined on

$$\mathcal{D}(T^*) \ := \ \{\psi \in \mathcal{H} \,|\, \exists \eta \in \mathcal{H} \,\text{s.t.}\, \langle \psi, T\varphi = \langle \eta, \varphi \rangle \forall \varphi \in \mathcal{H}\} \tag{1.1.6}$$

and whose action is

$$T^*\psi = \eta \,. \tag{1.1.7}$$

Definition 1.1.4. A linear operator T is said to be *self-adjoint* if $T = T^*$, and *essentially self-adjoint* if $\overline{T} = T^*$.

An operator T is said to be *symmetric* if

$$\langle T\psi, \varphi \rangle = \langle \psi, T\varphi \rangle \tag{1.1.8}$$

for al $\psi, \varphi \in \mathcal{D}(T)$.

A densely defined symmetric operator is always closable.

1.2 Minimal and maximal realisations

There are many standard ways to realise operators on Hilbert spaces out of formal differential operators. In this Section we present the choice adopted in this thesis.

Let $\widetilde{T}$ be a *formal differential operator* of order m with C^∞ coefficients a_α on an open set $\Omega \subset \mathbb{R}^d$:

$$\widetilde{T} \ = \ \sum_{|\alpha| \leqslant m} a_\alpha(x) D^\alpha \tag{1.2.1}$$

where $\alpha \in \mathbb{N}^m$ is a multi-index, $\alpha = (\alpha_1, \ldots, \alpha_m)$, $|\alpha| = \alpha_1 + \cdots + \alpha_m$ and $D^\alpha = (-\mathrm{i})^{|\alpha|} \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_m}}{\partial x_m^{\alpha_m}}$.

Its *formal adjoint* is the formal differential operator

$$T^\dagger \ = \ \sum_{|\alpha| \leqslant m} a_\alpha^\dagger(x) D^\alpha \tag{1.2.2}$$

where the coefficients $a_\alpha^\dagger(x)$ are defined from the relation

$$\sum_{|\alpha| \leqslant m} D^\alpha(\overline{a_\alpha(x)}u(x)) \ = \ \sum_{|\alpha| \leqslant m} a_\alpha^\dagger(x)(D^\alpha u)(x) \tag{1.2.3}$$

for any $u \in C_0^\infty(\Omega)$. A formal differential operator will be *formally self-adjoint* if $a_\alpha^\dagger(x) = a_\alpha(x)$ $\forall x \in \Omega$.

Note that if $\widetilde{T}$ is a formal differential operator of order m, so is its formal adjoint.

In the framework of quantum mechanics, one is mainly interested in a *rigorous definition* of operators of the form (1.2.1), on the Hilbert space $L^2(\Omega)$.

The information needed for such a definition is the *domain*, i.e. a vector subspace of $L^2(\Omega)$ where the action of the formal differential operator is well-defined. In this thesis we consider only *densely defined* operators, that are operators whose domain is a dense vector subspace of $L^2(\Omega)$. A first definition is a 'weak' realisation of the formal differential operator $\widetilde{T}$.

Definition 1.2.1. Given a formal differential operator of order m, $\widetilde{T} = \sum_{|\alpha| \leqslant m} a_\alpha(x) D^\alpha$, we define its *maximal* realisation on $L^2(\Omega)$ as the operator with domain

$$\mathcal{D}(T_{\max}) \;=\; \left\{ u \in L^2(\Omega) \,\Big|\, \begin{array}{c} \exists \eta \in L^2(\Omega) \quad \text{s.t.} \\ \langle u, \widetilde{T}^\dagger v \rangle = \langle \eta, v \rangle, \, \forall v \in C_0^\infty(\Omega) \end{array} \right\} \tag{1.2.4}$$

and action

$$T_{\max} u \;=\; \eta \,. \tag{1.2.5}$$

To check the well-posedness of this definition one has to check that $\mathcal{D}(T_{\max})$ is dense in $L^2(\Omega)$ and that η is defined uniquely. Both issues are consequences of the density of $C_0^\infty(\Omega)$ in $L^2(\Omega)$ (see e.g. [80, Lemma 2.19]) together with the fact that if $u \in C_0^\infty(\Omega)$, $T_{\max} u \in C_0^\infty(\Omega)$, and hence $C_0^\infty(\Omega) \subset \mathcal{D}(T_{\max})$. It follows from definition that $T_{\max}$ is a closed operator.

Definition 1.2.2. Given a formal differential operator of order m, $\widetilde{T} = \sum_{|\alpha| \leqslant m} a_\alpha(x) D^\alpha$, we define its *minimal* realisation $T_{\min}$ on $L^2(\Omega)$ as

$$(T_{\min} u)(x) \;=\; \sum_{|\alpha| \leqslant m} a_\alpha(x)(D^\alpha u)(x)$$
$$\mathcal{D}(T_{\min}) \;=\; \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{\widetilde{T}}} \,. \tag{1.2.6}$$

where the closure is intended in the graph norm of $\widetilde{T}$: $\|f\|_{\widetilde{T}}^2 = \|f\|^2 + \|\widetilde{T} f\|^2$.

To check the well-posedness of this definition one has to ensure that the operator defined on $C_0^\infty(\Omega)$ is closable. This is always the case, as their maximal realisation provide a closed extension.

We now state in the following Lemma some properties whose proof follows straightforwardly from the two definitions above. We refer to e.g. [60, Chapter 4] for the details of the proof.

Lemma 1.2.3. *Let $\widetilde{T}$ be a formal differential operator of order m, then*

   i) T_{min} and T_{max} are closed operators

   ii) $T_{min} \subset T_{max}$ in the sense of operator inclusion, and this means that T_{max} is densely defined;

   iii) $T_{max} = (T_{min}^\dagger)^*$, whence T_{max} is closed;

   iv) if $\widetilde{T}$ is formally self-adjoint, then $T_{min}^* = T_{max}$ and T_{min} is symmetric.

Remark 1.2.4. In the literature one often refers to realisations like the minimal one as *strong* realisations and to realisations like the maximal one as the *weak* realisations. These names are motivated by the interpretation of the derivatives appearing in the formal expression. The formal derivatives are intended as a classical derivatives in the first case and as weak derivatives in the second case.

One can find many other strong realisations of a formal differential operator of order m. Example of possible choices for their domain are $C_0^m(\Omega)$ or $C^m(\Omega) \cap L^2(\Omega)$.

1.3   Summary of von Neumann's vs Kreĭn's extension theory

The material of this Section is completely classical and stems from the original works of von Neumann [113], Stone [108], Friedrichs [45], and Kreĭn [74]. We give here a concise summary from a more modern perspective (see, e.g., [95, 104]) that includes also the Ando-Nishio characterisation of the Kreĭn-von Neumann extension (first obtained in the work of Ando and Nishio [6] and later generalised by Coddington and de Snoo [29], and by Prokaj, Sebestyén, and Stochel [106, 94, 107]) as well as Kadison's characterisation of the Friedrichs extension [67].

Roughly speaking, von Neumann's theory can be regarded as the "complex version" and Kreĭn's theory as the "real version" of the same idea, that consists of checking whether a complex number w is *real* by seeing whether $\frac{w-\mathrm{i}}{w+\mathrm{i}}$ is a phase (complex version), or alternatively checking whether w is *real positive* by seeing whether $\frac{w-1}{w+1}$ lies in $[-1, 1)$ (real version), based on the fact that $w \mapsto \frac{w-\mathrm{i}}{w+\mathrm{i}}$ is a bijection of the real axis onto the complex unit circle without the point 1, and that $w \mapsto \frac{w-1}{w+1}$ is a bijection of the non-negative half-line onto the interval $[-1, 1)$.

1.3.1   von Neumann's theory

Fixed $z \in \mathbb{C}\backslash\mathbb{R}$ and a Hilbert space $\mathcal{H}$, the Cayley transform

$$S \mapsto V_S := (S - z\mathbb{1})(S - \overline{z}\mathbb{1})^{-1}, \qquad \mathcal{D}(V_S) = \mathrm{ran}(S - \overline{z}\mathbb{1}), \tag{1.3.1}$$

is a bijective map of the set of densely defined symmetric operators on $\mathcal{H}$ onto the set of all isometric (i.e., norm-preserving) operators V on $\mathcal{H}$ for which $\mathrm{ran}(\mathbb{1} - V)$ is dense in $\mathcal{H}$. One has

$$\mathrm{ran}(\mathbb{1} - V_S) = \mathcal{D}(S). \tag{1.3.2}$$

S is closed if and only if V_S is, and if S' is another symmetric operator on $\mathcal{H}$, then $S \subset S'$ if and only if $V_S \subset V_{S'}$. The inverse map is the inverse Cayley transform

$$V \mapsto S_V := (z\mathbb{1} - \overline{z}V)(\mathbb{1} - V)^{-1}. \tag{1.3.3}$$

As a consequence, a densely defined symmetric operator S is self-adjoint if and only if its Cayley transform V_S is unitary: indeed, $S = S^*$ if and only if $\mathcal{H} = \mathrm{ran}(S - z\mathbb{1}) = \mathrm{ran}(S - \overline{z}\mathbb{1})$, which is equivalent to $\mathcal{H} = \mathrm{ran}(V_S) = \mathcal{D}(V_S)$.

Thus, finding a self-adjoint extension of S, call it $\widetilde{S}$, is equivalent to finding a unitary extension of V_S, which turns out to be $V_{\widetilde{S}}$, and this is in turn equivalent to (taking the operator closure and) finding a unitary operator from $\mathcal{D}(V_S)^\perp$ to $(\mathrm{ran}V_S)^\perp$, i.e., from $\ker(S^* - z\mathbb{1})$ to $\ker(S^* - \overline{z}\mathbb{1})$. This way the isometric V_S is extended to the unitary $V_{\widetilde{S}}$ on the whole $\mathcal{H}$ so that

$$V_S : \overline{\mathrm{ran}(S - \overline{z}\mathbb{1})} \xrightarrow{\cong} \overline{\mathrm{ran}(S - z\mathbb{1})}$$
$$V_{\widetilde{S}} \upharpoonright \ker(S^* - z\mathbb{1}) : \ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \overline{z}\mathbb{1}). \tag{1.3.4}$$

Obviously, this is possible if and only if $\dim \ker(S^* - z\mathbb{1}) = \dim \ker(S^* - \overline{z}\mathbb{1})$.

For a generic densely defined symmetric operator S each of the two dimensions above is actually constant in z throughout each of the two complex half-planes.[1] This justifies the unambiguous (z-independent) terminology of "deficiency indices" of S.

When the condition of equal deficiency indices is matched, then from (1.3.2) and from $(\mathbb{1} - V_{\widetilde{S}}) = (\mathbb{1} - V_{\widetilde{S}}) \upharpoonright \mathcal{D}(V_S) + (\mathbb{1} - V_{\widetilde{S}}) \upharpoonright \mathcal{D}(V_S)^\perp$ one has

$$\mathcal{D}(\widetilde{S}) = \mathrm{ran}(\mathbb{1} - V_{\widetilde{S}}) = \mathcal{D}(\overline{S}) + (\mathbb{1} - V_{\widetilde{S}})\ker(S^* - z\mathbb{1}), \tag{1.3.5}$$

---

[1] In fact, this is a result of Krasnosel'skii and Kreĭn [75].

and on a generic $f + u - V_{\widetilde{S}}u$ in $\mathcal{D}(\widetilde{S})$ ($f \in \mathcal{D}(\overline{S})$, $u \in \ker(S^* - z\mathbb{1})$) the action of $\widetilde{S}$, in view of (1.3.3), gives

$$
\begin{aligned}
\widetilde{S}(f + u - V_{\widetilde{S}}u) &= \overline{S}f + (z\mathbb{1} - \overline{z}V_{\widetilde{S}})(\mathbb{1} - V_{\widetilde{S}})^{-1}(\mathbb{1} - V_{\widetilde{S}})u \\
&= \overline{S}f + zu - \overline{z}V_{\widetilde{S}}u \,.
\end{aligned}
\tag{1.3.6}
$$

Because of (1.3.4), $V_{\widetilde{S}}$ in the r.h.s. of (1.3.5) and of (1.3.6) has to be thought of as a unitary map $\ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \overline{z}\mathbb{1})$. Thus, summarising:

Theorem 1.3.1 (von Neumann's theorem on self-adjoint extensions)**.** *A densely defined symmetric operator S on a Hilbert space $\mathcal{H}$ admits self-adjoint extensions if and only if S has equal deficiency indices. In this case there is a one-to-one correspondence between the self-adjoint extensions of S and the isomorphisms between $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \overline{z}\mathbb{1})$, where $z \in \mathbb{C}\backslash\mathbb{R}$ is fixed and arbitrary. Each self-adjoint extension is of the form S_U for some $U : \ker(S^* - z\mathbb{1}) \xrightarrow{\cong} \ker(S^* - \overline{z}\mathbb{1})$, where*

$$
\begin{aligned}
\mathcal{D}(S_U) &= \mathcal{D}(\overline{S}) \dotplus (\mathbb{1} - U)\ker(S^* - z\mathbb{1}) \\
S_U(f + u - Uu) &= \overline{S}u + zu - \overline{z}Uu = S^*(f + u - Uu) \,.
\end{aligned}
\tag{1.3.7}
$$

For each S_U, the unitary U is the restriction to $\ker(S^* - z\mathbb{1})$ of the Cayley transform of S_U.

1.3.2 Friedrichs extension and Kreĭn-von Neumann extension

If a given densely defined symmetric operator S on a Hilbert space $\mathcal{H}$ is *bounded below*, then it surely admits self-adjoint extensions (see, e.g., [95], Corollary to Theorem X.1). In fact, in this case S has two distinguished extensions (possibly coinciding), the Friedrichs extension and Kreĭn-von Neumann extension.

Theorem 1.3.2 (Friedrichs extension)**.** *Let S be a semi-bounded and densely defined symmetric operator on a Hilbert space $\mathcal{H}$.*

(i) *The form $(f, g) \mapsto \langle f, Sg \rangle$ with domain $\mathcal{D}(S)$ is closable. Its closure is the form whose domain, denoted by $\mathcal{D}[S]$, is given by the completion of $\mathcal{D}(S)$ with respect to the norm $f \mapsto \langle f, Sf \rangle + (1 - m(S))\|f\|^2$, where $m(S)$ is the bottom of S, and whose value $S[f, g]$ on any two $f, g \in \mathcal{D}[S]$ is given by $S[f, g] = \lim_{n \to \infty} \langle f_n, Sg_n \rangle$, where $(f_n)_n$ and $(g_n)_n$ are two sequences in $\mathcal{D}(S)$ that converge, respectively, to f and g in the above norm.*

(ii) *The form $(S[\cdot], \mathcal{D}[S])$ is bounded below and closed. Therefore, the operator associated with $(S[\cdot], \mathcal{D}[S])$ is self-adjoint. It is called the Friedrichs extension of S and denoted by S_F. By definition*

$$
\begin{aligned}
\mathcal{D}(S_F) &= \left\{ f \in \mathcal{D}[S] \,\middle|\, \begin{array}{l} \exists\, u_f \in \mathcal{H} \text{ such that} \\ S[f, g] = \langle u_f, g \rangle \ \forall g \in \mathcal{D}[S] \end{array} \right\} \\
S_F f &:= u_f \,.
\end{aligned}
\tag{1.3.8}
$$

(iii) *S_F is a bounded below self-adjoint extension of S with the same greatest lower bound as S, i.e.,*

$$
m(S_F) = m(S) \,,
\tag{1.3.9}
$$

and whose associated quadratic form coincides with the closure if the form $(f, g) \mapsto \langle f, Sg \rangle$ considered in (i)-(ii), i.e.,

$$
\mathcal{D}[S_F] = \mathcal{D}[S] \,, \qquad S_F[f, g] = S[f, g] \,.
\tag{1.3.10}
$$

(iv) $\mathcal{D}(S_F) = \mathcal{D}(S^*) \cap \mathcal{D}[S]$ and $S_F = S^* \upharpoonright \mathcal{D}[S]$.

(v) S_F is the only self-adjoint extension of S whose operator domain is contained in $\mathcal{D}[S]$.

(vi) If $\widetilde{S}$ is another bounded below self-adjoint extension of S, then $S_F \geqslant \widetilde{S}$.

(vii) $(S + \lambda\mathbb{1})_F = S_F + \lambda\mathbb{1}$ for $\lambda \in \mathbb{R}$.

Theorem 1.3.3 (Friedrichs extension – Kadison's construction [67])**.** *Let S be a semi-bounded, closed, and densely defined symmetric operator on a Hilbert space $\mathcal{H}$.*

(i) *The inner product $(f, g) \mapsto \langle f, Sg \rangle + (1 - m(S))\langle f, g \rangle$ on $\mathcal{D}(S)$ is positive definite. The corresponding completion $\mathcal{D}'$ is a subspace of $\mathcal{H}$ (in fact, $\mathcal{D}' = \mathcal{D}[S]$) with $\|g\| \leqslant \|g\|_{\mathcal{D}'}$.*

(ii) *For each $g \in \mathcal{H}$, the functional $f \mapsto \langle g, f \rangle$ on $\mathcal{D}(S)$ extends to a bounded linear functional on $(\mathcal{D}', \| \|_{\mathcal{D}'})$ with norm not exceeding $\|g\|$, and consequently $\exists\, ! \, g' \in \mathcal{D}(S^*) \cap \mathcal{D}'$ such that*

$$\langle g, f \rangle \;=\; \langle g', (S + \mathbb{1} - m(S)\mathbb{1})f \rangle \;=\; \langle g', f \rangle_{\mathcal{D}'} \qquad \forall f \in \mathcal{D}(S)\,.$$

The map $g \mapsto g'$ is realised by a linear operator K (i.e., $g' = Kg$) such that $K \in \mathcal{B}(\mathcal{H})$, $\|K\| \leqslant 1$, $K \geqslant \mathbb{O}$, and K is injective.

(iii) *The operator $S_K := K^{-1} - \mathbb{1} + m(S)\mathbb{1}$ is a self-adjoint extension of S with $m(S_K) = m(S)$ and $\mathcal{D}(S_K) \subset \mathcal{D}'$. It is the unique extension of S satisfying the last two properties.*

By comparison with Theorem 1.3.2(v) one has that S_K is precisely the Friedrichs extension of S: $S_K = S_F$.

Corollary 1.3.4. *Under the assumptions of Theorem 1.3.3, the Friedrichs extension S_F ($= S_K$) of S is characterised by*

$$\mathcal{D}(S_F) \;=\; \left\{ g' \in \mathcal{H} \,\middle|\, \begin{array}{c} \langle g', (S + \mathbb{1} - m(S)\mathbb{1})f \rangle = \langle g, f \rangle \ \ \forall f \in \mathcal{D}(S) \\ \text{for some } g \in \mathcal{H} \end{array} \right\} \tag{1.3.11}$$
$$\langle S_F g', f \rangle \;=\; \langle g', Sf \rangle \quad \forall f \in \mathcal{D}(S)\,, \quad \forall g' \in \mathcal{D}(S_F)\,.$$

The uniqueness of the Friedrichs extension (in the sense of Theorem 1.3.2(v) or Theorem 1.3.3(iii)) implies the additional noticeable property that follows. It is through this property that the Friedrichs extension plays a crucial, albeit somewhat hidden, role in the Tomita-Takesaki duality theory for von Neumann algebras and positive cones [110, §15].

Proposition 1.3.5 (The Friedrichs extension preserves the affiliation with a von Neumann algebra)**.**

(i) *Let S be a closed, densely defined, and positive symmetric operator on a Hilbert space $\mathcal{H}$ and let S_F its Friedrichs extension. If U is a unitary operator on $\mathcal{H}$ that commutes with S, in the sense that $U\mathcal{D}(S) \subset \mathcal{D}(S)$ and $USU^* = S$ on $\mathcal{D}(S)$, then U commutes with all the spectral projections of S_F.*

(ii) *More generally, if S is a closed, densely defined, and positive symmetric operator on a Hilbert space $\mathcal{H}$ affiliated [2] with a von Neumann algebra $\mathfrak{M}$ on $\mathcal{H}$, then its Friedrichs extension S_F too is affiliated with $\mathfrak{M}$.*

---

[2] By definition a closed and densely defined operator S on a Hilbert space $\mathcal{H}$ is affiliated with a von Neumann algebra $\mathfrak{M}$ on $\mathcal{H}$ when for any unitary $U \in \mathfrak{M}'$ (the commutant of $\mathfrak{M}$) one has $U\mathcal{D}(S) \subset \mathcal{D}(S)$ and $USU^* = S$ on $\mathcal{D}(S)$.

The Friedrichs extension of S is a form construction, obtained canonically given the datum S. In contrast, the Kreĭn-von Neumann extension of S is relative to a chosen reference lower bound to the bottom of S. Up to a trivial shift $S \mapsto S + \lambda \mathbb{1}$ for $\lambda \geqslant 0$ sufficiently large, one can always assume S to be a positive and densely defined symmetric operator and the reference lower bound to be zero.

Theorem 1.3.6 (Kreĭn-von Neumann extension)**.** *Let S be a positive and densely defined symmetric operator on a Hilbert space $\mathcal{H}$.*

(i) *Among all positive self-adjoint extensions of S there exists a unique smallest extension S_N in the sense of the operator ordering, that is, a unique extension with the property that $\widetilde{S} \geqslant S_N$ for any positive self-adjoint extension $\widetilde{S}$ of S. It is called the Kreĭn-von Neumann extension.*

(ii) *One has*

$$\begin{aligned} \mathcal{D}(S_N) &= \mathcal{D}(\overline{S}) + \ker S^* \\ S_N(f + u) &= \overline{S}f \qquad \forall f \in \mathcal{D}(\overline{S}),\ \forall u \in \ker S^* \end{aligned}$$

(1.3.12)

and (recall that $\mathcal{D}[S] = \mathcal{D}[S_F]$)

$$\begin{aligned} \mathcal{D}[S_N] &= \mathcal{D}[S_F] + \ker S^* \\ S_N[f + u, f' + u'] &= S_F[f, f'] \qquad \forall f, f' \in \mathcal{D}[S_F],\ \forall u, u' \in \ker S^*. \end{aligned}$$

(1.3.13)

In particular, $S_N u = 0\ \forall u \in \ker S^*$.

(iii) *If, in addition, S has positive bottom ($m(S) > 0$), then the sums in (1.3.12) and (1.3.13) are direct, that is,*

$$\begin{aligned} \mathcal{D}(S_N) &= \mathcal{D}(\overline{S}) \,\dot{+}\, \ker S^* \\ \mathcal{D}[S_N] &= \mathcal{D}[S_F] \,\dot{+}\, \ker S^*, \end{aligned}$$

(1.3.14)

and S_N is the only positive self-adjoint extension of S satisfying the two properties $\ker S^* \subset \mathcal{D}(S_N)$ and $S_N u = 0\ \forall u \in \ker S^*$.

Theorem 1.3.7 (Kreĭn-von Neumann extension: Ando-Nishio version)**.** *Let S be a positive and densely defined symmetric operator on a Hilbert space $\mathcal{H}$.*

(i) *The linear space*

$$\mathcal{E}(S) := \left\{ g \in \mathcal{H} \ \middle|\ \begin{array}{c} \exists\, c_g \geqslant 0 \text{ such that} \\ |\langle g, Sf \rangle|^2 \leqslant c_g \langle f, Sf \rangle\ \forall f \in \mathcal{D}(S) \end{array} \right\}$$

(1.3.15)

contains $\mathcal{D}(S)$ as well as the domain of any positive symmetric extension of S, in particular the domain of the Friedrichs extension S_F. $\mathcal{E}(S)$ is therefore dense in $\mathcal{H}$.

(ii) *The Kreĭn-von Neumann extension S_N of S satisfies*

$$\begin{aligned} \mathcal{D}[S_N] &= \mathcal{D}(S_N^{1/2}) = \mathcal{E}(S) \\ S_N[g] &= \|S_N^{1/2} g\|^2 = \nu(g) \end{aligned}$$

(1.3.16)

where $\nu(g) :=$ the smallest number c_g satisfying, for $g \in \mathcal{E}(S)$, the property $|\langle g, Sf \rangle|^2 \leqslant c_g \langle f, Sf \rangle\ \forall f \in \mathcal{D}(S)$.

Remark 1.3.8. One has $\nu(g) = \langle g, Sg \rangle\ \forall g \in \mathcal{D}(S)$ and $\nu(g) = 0\ \forall g \in \ker S^*$, consistently with (1.3.13) above.

Theorem 1.3.7 above has a counterpart when S is positive and symmetric with no a priori assumption on the density of $\mathcal{D}(S)$ in $\mathcal{H}$. In this case elementary counter-examples (see, e.g., [104, Example 13.2]) show that symmetry plus semi-boundedness of S is not enough to claim the existence of the Friedrichs extension or any other positive self-adjoint extension. On the other hand, there is a class of positive symmetric operators on $\mathcal{H}$, with possibly neither dense nor closed domain, for which it is crucial for general theoretical purposes to have conditions that ensure the existence of positive self-adjoint extensions: this is the class of shifted Kreĭn transforms of positive and densely defined symmetric operators on $\mathcal{H}$, see Section 1.3.3. Whence the relevance of the following result.

Theorem 1.3.9 (Ando-Nishio bound and existence theorem)**.** *Let S be a positive symmetric operator on a Hilbert space $\mathcal{H}$ whose domain is not necessarily a dense or a closed subspace of $\mathcal{H}$.*

  (i) *S admits a positive self-adjoint extension on $\mathcal{H}$ if and only if the set $\mathcal{E}(S)$ defined in (1.3.15) is dense in $\mathcal{H}$.*

  (ii) *For given $\gamma > 0$, S has a bounded positive self-adjoint extension $\widetilde{S}$ on $\mathcal{H}$ such that $\|\widetilde{S}\| \leqslant \gamma$ if and only if $\|Sf\|^2 \leqslant \gamma \langle f, Sf \rangle$ for all $f \in \mathcal{D}(S)$.*

1.3.3 Kreĭn's theory

Unlike von Neumann's theory, Kreĭn's extension theory only deals with densely defined symmetric operators that are *semi-bounded*. In this case the *existence* of self-adjoint extension(s) is not an issue, as proved by Stone [108, Theorem 9.21] and Friedrichs [45]. In fact, in terms of the tools of von Neumann's theory, semi-boundedness implies the coincidence of the two deficiency indices.[3]

The Kreĭn transform

$$S \mapsto K_S := (S - \mathbb{1})(S + \mathbb{1})^{-1}, \qquad \mathcal{D}(K_S) := \operatorname{ran}(S + \mathbb{1}), \qquad (1.3.17)$$

is a bijective map of the set of all positive symmetric operators on a Hilbert space $\mathcal{H}$ onto the set of all bounded symmetric operators K on $\mathcal{H}$ for which $\|K\| \leqslant 1$ and $\ker(\mathbb{1} - K) = \{0\}$, where for the operators of both sets the domain is possibly neither densely defined nor closed. In particular, if S is unbounded, then $\|K_S\| = 1$. The inverse map is the inverse Kreĭn transform

$$K \mapsto S_K := (\mathbb{1} + K)(\mathbb{1} - K)^{-1}, \qquad \mathcal{D}(S_K) = \operatorname{ran}(\mathbb{1} - K). \qquad (1.3.18)$$

In terms of the Kreĭn transform, S is self-adjoint if and only if K_S is self-adjoint. The Kreĭn transform preserves the operator inclusion:

$$S_1 \subset S_2 \;\Rightarrow\; K_{S_1} \subset K_{S_2}, \qquad (1.3.19)$$

and on self-adjoint operators it preserves the operator ordering:

$$S_1 = S_1^*, \; S_2 = S_2^*, \text{ and } S_1 \geqslant S_2 \;\;\Rightarrow\;\; K_{S_1} \geqslant K_{S_2}. \qquad (1.3.20)$$

Theorem 1.3.10 (Kreĭn's theorem on self-adjoint extensions)**.** *Let S be a densely defined and positive symmetric operator on a Hilbert space $\mathcal{H}$. Assume further that S is unbounded (otherwise the only self-adjoint extension of S is its operator closure $\overline{S}$).*

---

[3]The coincidence of the two deficiency indices of a semi-bounded and densely defined symmetric operator is a classical result (see, e.g., the first corollary to Theorem X.1 in [95]) which is a direct consequence of the above-mentioned Krasnosel'skii-Kreĭn result [75] on the constance of the deficiency indices throughout each of the two complex half-planes. In fact, such an argument is more general and proves as well the coincidence of the deficiency indices of a symmetric and densely defined operator S such that $\overline{S}$ has a real point in its resolvent set (see, e.g., the second corollary to Theorem X.1 in [95]). It is worth highlighting that the existence of a self-adjoint extension of a symmetric and densely defined S with a real point in the resolvent set of $\overline{S}$ is an independent result, proved first by Calkin [25] and later re-proved by Kreĭn [74].

(i) *There is a one-to-one correspondence between the positive self-adjoint extensions of S and the self-adjoint extensions $\widetilde{K}$ of the Kreĭn transform K_S that are bounded with $\|\widetilde{K}\| = 1$. For each such $\widetilde{K}$ one necessarily has $\ker(\mathbb{1} - \widetilde{K}) = \{0\}$, which makes the inverse Kreĭn transform of $\widetilde{K}$ well defined. Any such $\widetilde{K}$ identifies, via its inverse Kreĭn transform, a positive self-adjoint extension $\widetilde{S}$ of S (that is, $\widetilde{K} = K_{\widetilde{S}}$), and any positive self-adjoint extension of S is of this form.*

(ii) *The family of the self-adjoint extensions $\widetilde{K}$ of K_S with $\|\widetilde{K}\| = 1$ admits two elements, $K_{S,F}$ and $K_{S,N}$, such that a self-adjoint operator $\widetilde{K}$ belongs to this family if and only if $K_{S,N} \leqslant \widetilde{K} \leqslant K_{S,F}$. The corresponding inverse Kreĭn transforms of $K_{S,F}$ and $K_{S,N}$ are two positive self-adjoint extensions of S, respectively S_F and S_N, such that a self-adjoint operator $\widetilde{S}$ is a positive self-adjoint extension of S if and only if $S_N \leqslant \widetilde{S} \leqslant S_F$. S_F and S_N are nothing but the Friedrichs and the Kreĭn-von Neumann extensions of S (where the latter is defined with respect to the value zero as a reference lower bound), as given by Theorems 1.3.2 and 1.3.6.*

(iii) *In the special case when S has* positive bottom *($m(S) > 0$), for any semi-bounded self-adjoint extension $\widetilde{S}$ of S one has*

$$\mathcal{D}[\widetilde{S}] = \mathcal{D}[S_F] + \mathcal{D}[\widetilde{S}] \cap \ker S^*$$
$$\widetilde{S}[f + u, f' + u'] = S_F[f, f'] + \widetilde{S}[u, u'] \tag{1.3.21}$$
$$\forall f, f' \in \mathcal{D}[S_F], \ \forall u, u' \in \mathcal{D}[\widetilde{S}] \cap \ker S^*.$$

In particular,

$$\widetilde{S}[f, u] = 0 \qquad \forall f \in \mathcal{D}[S_F], \quad \forall u \in \mathcal{D}[\widetilde{S}] \cap \ker S^* \tag{1.3.22}$$

and

$$\widetilde{S} \geqslant 0 \qquad \Leftrightarrow \qquad \widetilde{S}[u, u] \geqslant 0 \quad \forall u \in \mathcal{D}[\widetilde{S}] \cap \ker S^*. \tag{1.3.23}$$

The sum in (1.3.21) *is direct for any* positive *self-adjoint extension of S:*

$$\mathcal{D}[\widetilde{S}] = \mathcal{D}[S_F] \dotplus \mathcal{D}[\widetilde{S}] \cap \ker S^* \qquad (m(S) > 0, \ m(\widetilde{S}) \geqslant 0). \tag{1.3.24}$$

Remark 1.3.11. In part (iii) of Theorem 1.3.10 above one actually first establishes (1.3.22), which is an independent result, valid for any semi-bounded extension of a bottom-positive and densely defined symmetric operator S (see, e.g., [74, Lemma 8]). This automatically implies $\widetilde{S}[f+u, f'+u'] = S_F[f, f'] + \widetilde{S}[u, u']$ in (1.3.21). The decomposition $\mathcal{D}[\widetilde{S}] = \mathcal{D}[S_F] + \mathcal{D}[\widetilde{S}] \cap \ker S^*$ in (1.3.21) requires an additional analysis, but in the special case of *positive* self-adjoint extensions it is a straightforward consequence of $S_N \leqslant \widetilde{S} \leqslant S_F$ given by part (ii) and of the property (1.3.13) for the domain of S_N. In the general case of *semi-bounded* extensions, the route to $\mathcal{D}[\widetilde{S}] = \mathcal{D}[S_F] + \mathcal{D}[\widetilde{S}] \cap \ker S^*$ (see, e.g., [74, Lemma 7 and Theorem 15]), goes through (1.3.13) again and the structural property

$$\mathcal{D}(S^*) = \mathcal{D}(S_F) \dotplus \ker S^* \qquad (m(S) > 0) \tag{1.3.25}$$

for the domain of S^*. For the relevance of the technique used to establish (1.3.25) we have included it, together with its proof, in the main part of this article (Section 2.1.2, Lemma 2.1.1).

Remark 1.3.12. Without the assumption $m(S) > 0$, the decomposition (1.3.21) for $\mathcal{D}[\widetilde{S}]$ fails to be true for arbitrary semi-bounded extensions of S: the inclusion $\mathcal{D}[\widetilde{S}] \supset \mathcal{D}[S_F] + \mathcal{D}[\widetilde{S}] \cap \ker S^*$ remains trivially valid, but can be proper.

Remark 1.3.13. The Kreĭn transform reduces the (difficult) problem of describing all positive self-adjoint extensions of S to the (possibly easier) problem of finding all the self-adjoint extensions of K_S with unit norm. The price, though, is that K_S is not necessarily densely defined in $\mathcal{H}$, which

makes the search for the "minimal" extension $K_{S,N}$ and the "maximal" extension $K_{S,F}$ of K_S on $\mathcal{H}$ different from the "ordinary" extension theory of densely defined symmetric operators.[4] A more explicit identification of $K_{S,N}$ and $K_{S,F}$ is due to Ando and Nishio [6] (and further developments) and proceeds as follows.

- One considers the positive symmetric operators $K^\pm := \mathbb{1} \pm K_S$ with common domain $\mathcal{D}(K_S)$.

- Although $\mathcal{D}(K_S)$ is not necessarily dense (which prevents one from introducing the Friedrichs extension), from the elementary inequality $\|K^\pm x\|^2 \leqslant 2\langle x, K^\pm x\rangle \ \forall x \in \mathcal{D}(K^\pm)$ one sees that they satisfy a Ando-Nishio bound as in Theorem 1.3.9(ii).

- Therefore, both K^+ and K^- admit a bounded positive self-adjoint extension on $\mathcal{H}$ with norm below 2, whence also (Theorem 1.3.6(ii)) the smallest positive self-adjoint extension $K_N^\pm$, for which $\|K_N^\pm\| \leqslant 2$ too.

- One then checks that among all the self-adjoint extensions $\widetilde{K}$ of K_S on $\mathcal{H}$ which are bounded with $\|\widetilde{K}\| = 1$, the extension $K_{S,N} := -(\mathbb{1} - K_N^+)$ is the smallest and $K_{S,F} := \mathbb{1} - K_N^-$ is the largest.

- The corresponding inverse Kreĭn transforms

$$
\begin{aligned}
S_N &= (\mathbb{1} + K_{S,N})(\mathbb{1} - K_{S,N})^{-1} \\
S_F &= (\mathbb{1} + K_{S,F})(\mathbb{1} - K_{S,F})^{-1}
\end{aligned}
\tag{1.3.26}
$$

  are self-adjoint extensions of S (Theorem 1.3.10(i)) that, because of (1.3.20), are, respectively, the Kreĭn-von Neumann and the Friedrichs extension of S.

As the distinction "Kreĭn vs KVB" may appear a somewhat artificial retrospective, let us emphasize the following. In Kreĭn's original work [74] each extension of S is proved to be bijectively associated with a self-adjoint extension, with unit norm, of the Kreĭn transform $(S - \mathbb{1})(S + \mathbb{1})^{-1}$ of S. This way, a difficult self-adjoint extension problem (extension of S) is shown to be equivalent to an easier one (extension of the Kreĭn transform of S), yet no general parametrisation of the extensions of S is given. The KVB theory provides in addition a parametrisation of the extensions, labelling each of them in the form S_B where B runs over all self-adjoint operators acting on Hilbert subspaces of $\ker(S^* + \lambda\mathbb{1})$, for some large enough $\lambda \geqslant 0$.

1.4 Weyl's limit-point limit-circle criterion

In this Section we review a useful classical criterion for computing deficiency indices for some first and second order ordinary differential operators. This criterion was first proposed by Weyl [120] for Sturm-Liouville operators many years before the Hilbert space approach to quantum mechanics and its extension to Dirac-like radial operators was first proposed by Roos and Sangren [100]. The proofs of the results can be found on standard textbooks on the subject, i.e. [104, Section 15.2], [95, Appendix X.I] or [119, Section 5].

The first class of ordinary differential operators we deal with is a sub-class of Sturm-Liouville operators sometimes referred as the class of one-dimensional Schrödinger operators. Their formal expression is

$$
\widetilde{T}_1 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)
\tag{1.4.1}
$$

for $x \in (a,b)$ with $-\infty \leqslant a < b \leqslant +\infty$ and the real valued potential $V \in C^0(a,b)$.

---

[4]The reader should be warned that, in this context, "minimal" and "maximal" are referred to the "minimal" and "maximal" self-adjoint extensions and not to the minimal and maximal realisations of Section 1.2.

Let $\lambda \in \mathbb{C}$. By a solution of the equation

$$\widetilde{T}_1 f - \lambda f \;=\; 0 \tag{1.4.2}$$

on (a,b) we mean a function f on (a,b) such that $f, f' \in AC[\alpha, \beta]$ for any compact $[\alpha, \beta] \subset (a,b)$ and $(\widetilde{T}_1 f)(x) - \lambda f(x) = 0$ for a.e. $x \in (a,b)$.

We say that a function $f : (a,b) \to \mathbb{C}$ is in L^2 near a if there exists $c \in (a,b)$ s.t. $f \in L^2(a,c)$. Analogously we say that f is in L^2 near b if there exists $c \in (a,b)$ such that $f \in L^2(c,b)$.

The second class of ordinary differential operator we deal with is a class of first-order differential operators with formal expression

$$\widetilde{T}_2 \;=\; -\mathrm{i}\sigma_2 \frac{\mathrm{d}}{\mathrm{d}x} + W(x) \tag{1.4.3}$$

where $W(x)$ is a Hermitian 2×2 matrix and σ_2 is the second Pauli matrix

$$\sigma_2 \;=\; \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} . \tag{1.4.4}$$

We require $W(x)$ to be continuous for $x \in (a,b)$ where $-\infty \leqslant a < b \leqslant +\infty$ and $\sigma_2 V(x)$ is traceless for any $x \in (a,b)$.

Analogously to the previous section, let $\lambda \in \mathbb{C}$. By a solution of the equation

$$\widetilde{T}_2 f - \lambda f \;=\; 0 \tag{1.4.5}$$

on (a,b) we mean a function f on (a,b) such that $f \in AC[\alpha, \beta]$ for any compact $[\alpha, \beta] \subset (a,b)$ and $(\widetilde{T}_2 f)(x) - \lambda f(x) = 0$ for a.e. $x \in (a,b)$.

We say that a function $f : (a,b) \to \mathbb{C}^2$ is in L^2 near a if there exists $c \in (a,b)$ such that $f \in L^2(a,c) \otimes \mathbb{C}^2$. Analogously we say that f is in L^2 near b if there exists $c \in (a,b)$ such that $f \in L^2(c,b) \otimes \mathbb{C}^2$.

From now on we refer to $\widetilde{T}$ as any of the formal differential expressions $\widetilde{T}_1$ or $\widetilde{T}_2$.

Theorem 1.4.1 (Weyl's alternative)**.** *Let d denote an end point of the interval (a,b). Then precisely one of the following two possibilities is valid:*

(i) For each $\lambda \in \mathbb{C}$, all solutions of (1.4.2) (or (1.4.5)) are in L^2 near d;

(ii) For each $\lambda \in \mathbb{C}$, there exists one solution of (1.4.2) (or (1.4.5)) which is not in L^2 near d.

In case (ii), for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there is a unique (up to a constant factor) nonzero solution of (1.4.2) (or (1.4.5)) which is in L^2 near d.

Definition 1.4.2. We say that $\widetilde{T}$ is in the *limit circle case* at d if case (i) holds, while $\widetilde{T}$ is in the *limit point case* at d if case (ii) holds.

Theorem 1.4.3. *The symmetric operator T_{min} has deficiency indices*

(2,2) if T is in the limit-circle case at both endpoints;

(1,1) if T is in the limit-circle case at one end point and in the limit point case at the other, and

(0,0) if T is in the limit point case at both endpoints.

As to conclude we state two useful criteria to check if an operator of the form (1.4.1) is in the limit-point or in the limit-circle case.

Proposition 1.4.4. *Let $b = +\infty$ and suppose that there exists $c, \gamma \in \mathbb{R}_+$ such that for all $x > c$, $V(x) > \gamma$. Then T is in the limit point case at $b = +\infty$.*

Proposition 1.4.5. *Suppose that $a = 0$ and $b \in (0, +\infty]$.*

(i) *If there exists a positive number c such that $c < b$ and $V(x) \geqslant \frac{3}{4}x^{-2}$ for all $x \in (0, c)$, then T is in the limit point case at $a = 0$.*

(ii) *If there are positive numbers ε and c such that $c < b$ and $|V(x)| \leqslant \left(\frac{3}{4} - \varepsilon\right)x^{-2}$ for all $x \in (0, c)$, then T is in the limit circle case at $a = 0$.*

Chapter 2

Kreĭn-Višik-Birman Self-adjoint Extension Theory

Beside that Kreĭn-Višik-Birman theory is nowadays an undoubtedly classical topic, and in fact to some extent even superseded by more modern mathematical techniques, it has several features that makes its use very convenient in the context of self-adjoint realisations of quantum mechanical Hamiltonians. In this framework, results from Kreĭn and Birman have been known since long to bring in this context complementary or also new information: one paradigmatic instance is the study of particle Hamiltonians of contact interaction carried on by trailblazers such as Berezin, Faddeev, and above all Minlos and his school [88, 85, 86] – an ample historical survey of which is in [84, Section 2].

The material of this chapter, which is essentially the content of my work [51], is written with the purpose to provide an exhaustive recapitulation of the KVB theory. Main results on classification of self-adjoint extensions are reproduced in Section 2.2. These statements are actually those by which (part of) the KVB theory has been presented, re-derived, discussed, and applied in the subsequent literature in English language.

In Section 2.3 we complete the main core of the theory with results that characterise relevant properties of the extensions, such as invertibility, semi-boundedness, and other special features of the negative discrete spectrum, in terms of the corresponding properties of the extension parameter.

In Section 2.4 we discuss, within the KVB formalism, the structure of resolvents of self-adjoint extensions, in the form of Kreĭn-like resolvent formulas. The results emerging from Sections 2.3 and 2.4 corroborates the picture that the KVB extension parametrisation is in many fundamental aspects more informative than von Neumann's parametrisation.

Last, in Section 2.5 we show how the general formulas of the KVB theory apply to simple examples in which the extension problem by means of von Neumann's theory is already well known, so as to make the comparison between the two approaches evident.

2.1 Decomposition of the domain of the adjoint

The two aims of this Section are to recall some useful results on the decomposition of the domain of the adjoint of a densely defined symmetric operator and to introduce some terminology. We skipped all proofs, for which the reader is referred to [51].

2.1.1   General assumptions. Choice of a reference lower bound.

In the following we shall assume that S is a semi-bounded (below), not necessarily closed, densely defined symmetric operator acting on a Hilbert space $\mathcal{H}$. Unlike the early developments of the theory (Kreĭn's theory), no restriction is imposed to the magnitude of the deficiency indices $\dim \ker(S^* \pm \mathrm{i})$ of S: in particular, they can also be infinite.

It is not restrictive to assume further

$$m(S) > 0 \,, \tag{2.1.1}$$

for in the general case one applies the discussion that follows to the strictly positive operator $S + \lambda \mathbb{1}$, $\lambda > -m(S)$, and then re-express trivially the final results in terms of the original S.

Associated to S are two canonical, distinguished self-adjoint extensions, the well-known *Friedrichs* extension S_F and *Kreĭn-von Neumann* extension S_N. Whereas a complete summary of the construction and of the properties of such extensions is presented in Section 1.3.2, which we will be making reference to whenever in the following we shall need a particular attribute of S_F or S_N for the proofs, let us recall here their distinguishing features.

The extension S_F is semi-bounded and with the same bottom $m(S_F) = m(S)$ of S. Its quadratic form is precisely the closure of the (closable) quadratic form associated with S. In fact, S_F is the restriction of S^* to the domain $\mathcal{D}[S] \cap \mathcal{D}(S^*)$. Among all self-adjoint extensions of S, S_F is *the only one* whose operator domain is contained in $\mathcal{D}[S]$, and moreover S_F is larger than any other semi-bounded extension $\widetilde{S}$ of S, in the sense of the ordering $S_F \geqslant \widetilde{S}$ (which, in particular, means $\mathcal{D}[S_F] \subset \mathcal{D}[\widetilde{S}]$).

Thus, *the choice $m(S) > 0$ implies that the Friedrichs extension S_F of S is invertible with bounded inverse defined everywhere on $\mathcal{H}$*: this will allow S_F^{-1} to enter directly the discussion. In the general case in which S_F is not necessarily invertible, the role of S_F^{-1} can be naturally replaced in many respects (but not all) by the inverse $\widetilde{S}^{-1}$ of any a priori known self-adjoint extension $\widetilde{S}$ of S, which thus takes the role of given "datum" of the theory.

With the choice $m(S) > 0$, the level 0 becomes naturally the reference value with respect to which to express the other distinguished (canonically given) extension of S, the Kreĭn-von Neumann extension S_N. It is qualified among all other positive self-adjoint extensions $\widetilde{S}$ of S by being the unique smallest, in the sense $\widetilde{S} \geqslant S_N$.

We underline that unlike Kreĭn's original theory and many of the recent presentations of the KVB theory, the discussion here is *not* going to be restricted to the positive self-adjoint extensions of S. On the contrary, we shall present the full theory that includes also those extensions, if any, with finite negative bottom, or even unbounded below.

2.1.2   Adjoint of a semi-bounded symmetric operator. Regular and singular part.

The first step of the theory is to describe the structure of the *domain of the adjoint S^** of S. Recall that a characterisation of $\mathcal{D}(S^*)$ is already given by von Neumann's formula

$$\mathcal{D}(S^*) \;=\; \mathcal{D}(\overline{S}) \dotplus \ker(S^* - z\mathbb{1}) \dotplus \ker(S^* - \overline{z}\mathbb{1}) \qquad \text{for } z \in \mathbb{C} \backslash \mathbb{R} \,, \tag{2.1.2}$$

which is valid, more generally, for any densely defined S. The KVB theory works with a "real" version of (2.1.2), with $z = 0$ and with the space

$$U \;:=\; \ker S^* \tag{2.1.3}$$

instead of the two deficiency spaces $\ker(S^* - z\mathbb{1})$ and $\ker(S^* - \overline{z}\mathbb{1})$. With a self-explanatory nomenclature, U shall henceforth be referred to as *the* deficiency space of S, with no restriction on $\dim U$.

The result consists of a decomposition of $\mathcal{D}(S^*)$ first proved by Kreĭn (see also Remark 1.3.11) and a further refinement, initially due to Višik, to which Birman gave later an alternative proof.

Lemma 2.1.1 (Kreĭn decomposition formula for $\mathcal{D}(S^*)$). *For a densely defined symmetric operator S with positive bottom,*

$$\mathcal{D}(S^*) = \mathcal{D}(S_F) \dotplus \ker S^*. \tag{2.1.4}$$

Theorem 2.1.2 (Višik-Birman decomposition formula for $\mathcal{D}(S^*)$). *For a densely defined symmetric operator S with positive bottom,*

$$\mathcal{D}(S^*) = \mathcal{D}(\overline{S}) \dotplus S_F^{-1} \ker S^* \dotplus \ker S^*. \tag{2.1.5}$$

Remark 2.1.3. The argument of the proof above can be repeated to conclude

$$\mathcal{D}(S_F) = \mathcal{D}(\overline{S}) \dotplus S_F^{-1} \ker S^*. \tag{2.1.6}$$

and hence

$$\mathcal{D}(S_F) \cap \ker S^* = \{0\}. \tag{2.1.7}$$

Indeed, while it is obvious that the r.h.s. of (2.1.6) is contained in the l.h.s., conversely one takes a generic $g \in \mathcal{D}(S_F)$ and decomposes $S_F g = h_0 + \widetilde{u}$ with $h_0 \in \overline{\operatorname{ran}S}$ and $\widetilde{u} \in U$ as above, whence, by the same argument, $g = S_F^{-1} h_0 + S_F^{-1} \widetilde{u}$ with $S_F^{-1} h_0 \in \mathcal{D}(\overline{S})$.

Remark 2.1.4. Precisely as in the remark above, one also concludes that

$$\mathcal{D}(\widetilde{S}) = \mathcal{D}(\overline{S}) \dotplus \widetilde{S}^{-1} \ker S^* \tag{2.1.8}$$

for any self-adjoint extension $\widetilde{S}$ of S that is invertible everywhere on $\mathcal{H}$.

Remark 2.1.5. Since S is closable and injective ($m(S) > 0$), then as well known

$$\overline{\operatorname{ran}S} = \operatorname{ran}\overline{S}. \tag{2.1.9}$$

Thus, in the above proof one could claim immediately that $h_0 = \overline{S}f$ for some $f \in \mathcal{D}(\overline{S})$, whence $S_F^{-1} h_0 = S_F^{-1} \overline{S} f = f \in \mathcal{D}(\overline{S})$.

Remark 2.1.6. In view of the applications in which S and S_F are differential operators on an L^2-space and hence $\mathcal{D}(S_F)$ indicates an amount of regularity of its elements, it is convenient to regard $\mathcal{D}(S_F) = \mathcal{D}(\overline{S}) \dotplus S_F^{-1} U$ in (2.1.5) as the "*regular component*" and, in contrast, $U = \ker S^*$ as the "*singular component*" of the domain of S^*.

Remark 2.1.7. In all the previous formulas the assumption $m(S) > 0$ only played a role to guarantee the existence of the everywhere defined and bounded operator S_F^{-1}. It is straightforward to adapt the arguments above to prove the following: if S is a symmetric and densely defined operator on $\mathcal{H}$ and $\widetilde{S}$ is a self-adjoint extension of S, then for any $z \in \rho(\widetilde{S})$ (the resolvent set of $\widetilde{S}$)

$$\mathcal{D}(S^*) = \mathcal{D}(\overline{S}) \dotplus (\widetilde{S} - z\mathbb{1})^{-1} \ker(S^* - \overline{z}\mathbb{1}) \dotplus \ker(S^* - z\mathbb{1}) \tag{2.1.10}$$

$$\mathcal{D}(S^*) = \mathcal{D}(\widetilde{S}) \dotplus \ker(S^* - z\mathbb{1}) \tag{2.1.11}$$

$$\mathcal{D}(\widetilde{S}) = \mathcal{D}(\overline{S}) \dotplus (\widetilde{S} - z\mathbb{1})^{-1} \ker(S^* - \overline{z}\mathbb{1}). \tag{2.1.12}$$

2.2 Formulations of the KVB theory

We are now in the condition of re-stating the main results of the KVB extension in the form they will be used later on. We omit the proofs, that can be found in our paper [51].

Theorem 2.2.1 (Classification of self-adjoint extensions – operator version). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$). There is a one-to-one correspondence between the family of all self-adjoint extensions of S on $\mathcal{H}$ and the family of the self-adjoint operators on Hilbert subspaces of $\ker S^*$. If T is any such operator, in the correspondence $T \leftrightarrow S_T$ each self-adjoint extension S_T of S is given by*

$$S_T \;=\; S^* \upharpoonright \mathcal{D}(S_T)$$
$$\mathcal{D}(S_T) \;=\; \left\{ f + S_F^{-1}(Tv + w) + v \;\middle|\; \begin{array}{l} f \in \mathcal{D}(\overline{S})\,,\; v \in \mathcal{D}(T) \\ w \in \ker S^* \cap \mathcal{D}(T)^{\perp} \end{array} \right\}. \qquad (2.2.1)$$

Theorem 2.2.2 (Characterisation of semi-bounded extensions). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$). If, with respect to the notation of (2.2.1), S_T is a self-adjoint extension of S, and if $\alpha < m(S)$, then*

$$\langle g, S_T g \rangle \;\geqslant\; \alpha \,\|g\|^2 \qquad \forall g \in \mathcal{D}(S_T)$$
$$\Updownarrow \qquad\qquad\qquad\qquad (2.2.2)$$
$$\langle v, Tv \rangle \;\geqslant\; \alpha\|v\|^2 + \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1} v \rangle \qquad \forall v \in \mathcal{D}(T)\,.$$

As an immediate consequence, $m(T) \geqslant m(S_T)$ for any semi-bounded S_T. In particular, positivity or strict positivity of the bottom of S_T is equivalent to the same property for T, that is,

$$\begin{aligned} m(S_T) \;\geqslant\; 0 &\quad \Leftrightarrow \quad m(T) \;\geqslant\; 0 \\ m(S_T) \;>\; 0 &\quad \Leftrightarrow \quad m(T) \;>\; 0\,. \end{aligned} \qquad (2.2.3)$$

Moreover, if $m(T) > -m(S)$, then

$$m(T) \;\geqslant\; m(S_T) \;\geqslant\; \frac{m(S)\,m(T)}{m(S) + m(T)}\,. \qquad (2.2.4)$$

Theorem 2.2.3 (Characterisation of semi-bounded extensions – form version). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$) and, with respect to the notation of (2.2.1), let S_T be a semi-bounded (not necessarily positive) self-adjoint extension of S. Then*

$$\mathcal{D}[T] \;=\; \mathcal{D}[S_T] \cap \ker S^* \qquad\qquad (2.2.5)$$

and

$$\begin{aligned} \mathcal{D}[S_T] \;&=\; \mathcal{D}[S_F] \,\dot{+}\, \mathcal{D}[T] \\ S_T[f + v, f' + v'] \;&=\; S_F[f, f'] + T[v, v'] \\ &\qquad \forall f, f' \in \mathcal{D}[S_F],\; \forall v, v' \in \mathcal{D}[T]\,. \end{aligned} \qquad (2.2.6)$$

As a consequence,

$$S_{T_1} \;\geqslant\; S_{T_2} \qquad \Leftrightarrow \qquad T_1 \;\geqslant\; T_2 \qquad\qquad (2.2.7)$$

and

$$T \;\geqslant\; S_T\,. \qquad\qquad (2.2.8)$$

Proposition 2.2.4 (Parametrisation of S_F and S_N). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$) and let S_T be a positive self-adjoint extension of S, parametrised by T according to Theorems 2.2.1 and 2.2.3.*

  (i) *S_T is the Friedrichs extension when $\mathcal{D}[T] = \{0\}$ ("$T = \infty$").*

  (ii) *S_T is the Kreĭn-von Neumann extension when $\mathcal{D}(T) = \mathcal{D}[T] = \ker S^*$ and $Tu = 0 \;\forall u \in \ker S^*$ ($T = \mathbb{O}$).*

Let us discuss in the last part of this Section yet another equivalent formulation of the general representation theorem for self-adjoint extensions.

Theorem 2.2.5 (Classification of self-adjoint extensions – operator version)**.** *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$). There is a one-to-one correspondence between the family of all self-adjoint extensions of S on $\mathcal{H}$ and the family of the self-adjoint operators on Hilbert subspaces of $\ker S^*$. If T is any such operator, $P_T : \mathcal{H} \to \mathcal{H}$ is the orthogonal projection onto $\overline{\mathcal{D}(T)}$, and $P_* : \mathcal{D}(S^*) \to \mathcal{D}(S^*)$ is the (non-orthogonal, in general) projection onto $\ker S^*$ with respect to Kreĭn's decomposition formula $\mathcal{D}(S^*) = \mathcal{D}(S_F) \dotplus \ker S^*$ (Lemma 2.1.1), then in the correspondence $T \leftrightarrow S_T$ each self-adjoint extension S_T of S is given by*

$$S_T \; = \; S^* \upharpoonright \mathcal{D}(S_T)$$
$$\mathcal{D}(S_T) \; = \; \left\{ g \in \mathcal{D}(S^*) \; \middle| \; \begin{array}{l} P_* g \in \mathcal{D}(T) \text{ and} \\ P_T S^* g = T P_* g \end{array} \right\}. \tag{2.2.9}$$

Proposition 2.2.6. *The parameter T in (2.2.9) is precisely the same as in (2.2.1), that is, the representation given in Theorem 2.2.5 is the same as the one given in Theorem 2.2.1. In other words, the two theorems are* equivalent*. In particular, given a self-adjoint extension $\widetilde{S}$ of S, its extension parameter T (i.e., the operator T for which $\widetilde{S} = S_T$) is the operator acting on the Hilbert space $\overline{P_* \mathcal{D}(\widetilde{S})}$ with domain $\mathcal{D}(T) = P_* \mathcal{D}(\widetilde{S})$ and action $T P_* g = P_T S_T g \; \forall g \in \mathcal{D}(\widetilde{S})$.*

2.3 Invertibility, semi-boundedness, and negative spectrum

In this Section we complete the discussion of the main results that can be proved within the KVB theory, focusing on the link between relevant features (such as invertibility, semi-boundedness, structure of the negative spectrum) of a self-adjoint extension of a given densely defined symmetric operator S with positive bottom, and the corresponding features of the extension parameter given by the theory. Such a close link allows one to appreciate even more the effectiveness of the KVB extension parameter, as compared to von Neumann's parametrisation. We adopt here the notation $T \leftrightarrow S_T$ for the parametrisation of the extensions – see Section 2.2.

A first link between S_T and T, which is straightforward although it is not explicitly present in Birman's original work, is the following.

Theorem 2.3.1 (Invertibility)**.** *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$) and let S_T be a generic self-adjoint extension of S according to the parametrisation (2.2.1) of Theorem 2.2.1. Then*

  (i) S_T is injective $\Leftrightarrow$ T is injective,

  (ii) S_T is surjective $\Leftrightarrow$ T is surjective,

 (iii) S_T is invertible on the whole $\mathcal{H}$ $\Leftrightarrow$ T is invertible on the whole $\overline{\mathcal{D}(T)}$.

Proof. Assume that S_T is injective and let $v \in \mathcal{D}(T)$ be such that $Tv = 0$. Then v is an element in $\mathcal{D}(S_T)$, because it is a vector of the form (2.2.1), $g = f + S_F^{-1}(Tv + w) + v$, with $f = w = 0$. Since $S_T v = 0$, by injectivity of S_T one concludes that $v = 0$. Conversely, if T is injective and for some $g = f + S_F^{-1}(Tv + w) + v \in \mathcal{D}(S_T)$ one has $S_T g = 0$, then $\overline{S} f + Tv + w = 0$. Since $\overline{S} f + Tv + w \in \mathrm{ran}\overline{S} \boxplus \mathrm{ran} T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$, one must have $\overline{S} f = Tv = w = 0$. Owing to the injectivity of $\overline{S}$ and T, $f = v = 0$ and hence $g = 0$. This completes the proof of (i). As for (ii), in the notation of (2.2.1) one has that $\mathrm{ran}\, S_T = \mathrm{ran}\overline{S} \boxplus \mathrm{ran} T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$ and in fact $\mathrm{ran}\overline{S} = \overline{\mathrm{ran}S}$ (Remark 2.1.5). Thus, T is surjective $\Leftrightarrow \mathrm{ran} T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \overline{\mathrm{ran} T} \oplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \ker S^*$ $\Leftrightarrow \mathrm{ran} S_T = \overline{\mathrm{ran}S} \oplus \ker S^* = \mathcal{H} \Leftrightarrow S_T$ is surjective. (iii) is an obvious consequence of (i) and (ii). $\square$

Remark 2.3.2. A generalisation of Theorems 2.3.1 and 2.4.4 for non semi-bounded operators with a spectral gap is Theorem 5.3.6.

Semi-boundedness is another relevant feature of the self-adjoint extensions that can be controlled in terms of the KVB extension parameter. The sub-family of the semi-bounded self-adjoint extensions of S is the object of Theorem 2.2.2. Here below we supplement the information of that theorem with the answer to the question on whether the semi-boundedness of S_T and of T are *equivalent*. This is another result that is not explicitly present in Birman's discussion, although it follows from it. As a consequence, we derive within the KVB theory the fact that when S has a finite deficiency index all its self-adjoint extensions are bounded below.

Theorem 2.3.3 (Semi-boundedness). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$), $P_K : \mathcal{H} \to \mathcal{H}$ be the orthogonal projection onto $\ker S^*$, and for each $\alpha < m(S)$ let*

$$M(\alpha) := P_K(\alpha \mathbb{1} + \alpha^2(S_F - \alpha \mathbb{1})^{-1})P_K = P_K(\alpha S_F(S_F - \alpha \mathbb{1})^{-1})P_K. \qquad (2.3.1)$$

Let S_T be a generic self-adjoint extension of S according to the parametrisation (2.2.1) of Theorem 2.2.1. Assume that $m(T) \in [-\infty, 0)$, that is, T is either unbounded below or with finite negative bottom (otherwise it is already known by (2.2.3) in Theorem 2.2.2 that $m(T) \geqslant 0 \Leftrightarrow m(S_T) \geqslant 0$). Then the two conditions

(i) S_T is bounded below (on $\mathcal{H}$)

(ii) T is bounded below (on $\overline{\mathcal{D}(T)}$)

are equivalent if and only if $M(\alpha)$ "diverges to $-\infty$ uniformly as $\alpha \to -\infty$", meaning that $\forall R > 0$ $\exists \alpha_R < 0$ such that $M(\alpha) \leqslant -R\mathbb{1}$ for each $\alpha \leqslant \alpha_R$.

Proof. Since (i) $\Rightarrow$ (ii) is always true (owing to (2.2.2) in Theorem 2.2.2), what must be proven is the equivalence between the implication (ii) $\Rightarrow$ (i) and the condition of uniform divergence to $-\infty$ for $M(\alpha)$. Assume (ii) $\Rightarrow$ (i), that is, assume that for arbitrary $R > -m(T)$ the condition $T \geqslant -R\mathbb{1}$ implies $S_T \geqslant \alpha_R \mathbb{1}$ for some $\alpha_R < 0$ and hence also $S_T \geqslant \alpha \mathbb{1}$ $\forall \alpha \leqslant \alpha_R$ (if the lower bound α_R was non-negative, then $m(T)$ would be non-negative too, against the assumption). In turn, owing to (2.2.2) and (2.3.1), $S_T \geqslant \alpha \mathbb{1}$ $\forall \alpha \leqslant \alpha_R$ is equivalent to $T \geqslant M(\alpha)$ $\forall \alpha \leqslant \alpha_R$. Then, for $T \geqslant -R\mathbb{1}$ to imply $T \geqslant M(\alpha)$ $\forall \alpha \leqslant \alpha_R$, necessarily $M(\alpha) \leqslant -R\mathbb{1}$ $\forall \alpha \leqslant \alpha_R$. Conversely, assume now that for arbitrary $R > 0$ there exists α_R such that $M(\alpha) \leqslant -R\mathbb{1}$ $\forall \alpha \leqslant \alpha_R$: we want to deduce (ii) $\Rightarrow$ (i). To this aim, assume that T is bounded below and apply the assumption for $R = -m(T)$: for the corresponding α_R one has $M(\alpha_R) \leqslant -R\mathbb{1} = m(T)\mathbb{1} \leqslant T$, which by (2.2.2) implies $S_T \geqslant \alpha_R\mathbb{1}$. $\square$

Corollary 2.3.4 (Finite deficiency index). *If S is a semi-bounded and densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with finite deficiency index, then*

(i) the semi-boundedness of S_T is equivalent to the semi-boundedness of T;

(ii) any self-adjoint extension of S is bounded below.

Proof. It is not restrictive to assume $m(S) > 0$ and hence $\dim \ker S^* < \infty$. Part (ii) follows from (i) because T is now defined on a finite-dimensional Hilbert space and is therefore bounded. Part (i) follows from Theorem 2.3.3 once one shows that $M(\alpha)$ diverges uniformly to $-\infty$. Irrespectively of whether $\dim \ker S^*$ is finite or not,

$$\lim_{\alpha \to -\infty} \langle u, M(\alpha)u \rangle = -\infty \qquad \forall u \in \ker S^*. \qquad (2.3.2)$$

Indeed, for any $u \in \ker S^*$ one has $u \notin \mathcal{D}[S_F]$ (see (1.3.14)), whence

$$\int_{[0,\,+\infty)} \lambda \, \mathrm{d}\langle u, E^{(S_F)}(\lambda)u \rangle \;=\; +\infty \,,$$

where $\mathrm{d}E^{(S_F)}$ denotes the spectral measure of S_F; therefore, since $\frac{\lambda\alpha}{\lambda-\alpha} \to -\lambda$ as $\alpha \to -\infty$,

$$\langle u, M(\alpha)u \rangle \;=\; \int_{[0,\,+\infty)} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle u, E^{(S_F)}(\lambda)u \rangle \;\xrightarrow{\;\alpha\to-\infty\;}\; -\infty \,.$$

Under the additional assumption $\dim \ker S^* < \infty$ let us now show that (2.3.2) implies a *uniform* divergence in the sense of Theorem 2.3.3. For arbitrarily fixed $R > 0$ decompose $u = f_R + v_R$ with

$$f_R \;:=\; E^{(S_F)}([0,2R])u \,, \qquad v_R \;:=\; E^{(S_F)}((2R,+\infty))u \,.$$

Observe that $f_R \in \mathcal{D}(S_F)$, because

$$\int_{[0,\,+\infty)} \lambda^2 \, \mathrm{d}\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \;=\; \int_{[0,\,2R]} \lambda^2 \, \mathrm{d}\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \;\leqslant\; 4R^2 \|f_R\|^2 \,,$$

while necessarily $v_R \notin \mathcal{D}(S_F)$ because $u \notin \mathcal{D}(S_F)$. One has

$$\begin{aligned}
\langle u, M(\alpha)u \rangle \;&=\; \langle u, M(\alpha)u \rangle \;=\; \int_{[0,\,+\infty)} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle u, E^{(S_F)}(\lambda)u \rangle \\
&=\; \int_{[0,\,2R]} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \;+\; \int_{(2R,\,+\infty)} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle v_R, E^{(S_F)}(\lambda)v_R \rangle \,.
\end{aligned}$$
(a)

In the second integral in the r.h.s above $\lambda > 2R$, whence $2R > \frac{2R\lambda}{2\lambda-2R}$: therefore, choosing $\alpha < -2R$ implies $-\alpha > \frac{2R\lambda}{2\lambda-2R}$ and the latter condition is equivalent to $\frac{\lambda\alpha}{\lambda-\alpha} < -R$, thus

$$\int_{(2R,\,+\infty)} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle v_R, E^{(S_F)}(\lambda)v_R \rangle \;<\; -R\,\|v_R\|^2 \qquad (\alpha < -2R) \,.$$
(b)

Let us now exploit the assumption $\dim \ker S^* = d$ for some $d \in \mathbb{N}$ in order to estimate the first integral in the r.h.s of (a). Obviously there is $d_R \in \mathbb{N}$, $d_R \leqslant d$, such that

$$\dim E^{(S_F)}([0,2R]) \ker S^* \;=\; d_R$$
(c)

and let $\{\varphi_{R,1}, \ldots, \varphi_{R,d_R}\}$ be an orthonormal basis of this d_R-dimensional subspace of $\mathcal{D}(S_F)$. Decompose $f_R = f_{R,1} + \cdots + f_{R,d_R}$ with $f_{R,j} := \langle \varphi_{R,j}, f_R \rangle \varphi_{R,j}$, $j = 1, \ldots, d_R$. Then

$$\begin{aligned}
\int_{[0,\,2R]} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \;&=\; \sum_{j=1}^{d_R} \int_{[0,\,2R]} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle f_{R,j}, E^{(S_F)}(\lambda)f_{R,j} \rangle \\
&=\; \sum_{j=1}^{d_R} |\langle \varphi_{R,j}, f_R \rangle|^2 \int_{[0,\,2R]} \frac{\lambda\,\alpha}{\lambda-\alpha} \, \mathrm{d}\langle \varphi_{R,j}, E^{(S_F)}(\lambda)\varphi_{R,j} \rangle \\
&=\; \sum_{j=1}^{d_R} |\langle \varphi_{R,j}, f_R \rangle|^2 \langle \widetilde{\varphi}_{R,j}, M(\alpha)\widetilde{\varphi}_{R,j} \rangle \,.
\end{aligned}$$

Where the $\widetilde{\varphi}_{R,j} \in \ker S^*$ are preimages under $E^{(S_F)}([0,2R])$ of the orthonormal basis, so that the last line just uses the fact that $E^{(S_F)}([0,2R])$ is a orthogonal projection. Owing to (2.3.2), each

$\langle \widetilde{\varphi}_{R,j}, M(\alpha)\widetilde{\varphi}_{R,j} \rangle$ diverges to $-\infty$ as $\alpha \to -\infty$: there is only a *finite* number of them (and it does not exceed d), so there is a common threshold $\alpha_R < 0$ such that

$$\sup_{j \in \{1,\dots,d_R\}} \langle \widetilde{\varphi}_{R,j}, M(\alpha)\widetilde{\varphi}_{R,j} \rangle \;\leqslant\; -R \qquad \forall \alpha \leqslant \alpha_R\,.$$

Therefore

$$\int\limits_{[0,\,2R]} \frac{\lambda\,\alpha}{\lambda - \alpha}\, \mathrm{d}\langle f_R, E^{(S_F)}(\lambda)f_R \rangle \;\leqslant\; -R\|f_R\|^2 \qquad (\alpha \leqslant \alpha_R) \tag{d}$$

(α_R only depends on R (and on d), *not* on f_R). Plugging the bounds (b) and (d) into (a) yields

$$\langle u, M(\alpha)u \rangle \;<\; -R\|f_R\|^2 - R\|v_R\|^2 \;=\; -R\|u\|^2$$

for $\alpha < \min\{-2R, \alpha_R\}$. From the arbitrariness of $u \in \ker S^*$ and of $R > 0$ one concludes that $M(\alpha) \to -\infty$ uniformly as $\alpha \to -\infty$. $\qquad\square$

Corollary 2.3.5. *If S is a semi-bounded and densely defined symmetric operator on a Hilbert space $\mathcal{H}$, whose bottom is positive ($m(S) > 0$) and whose Friedrichs extension has compact inverse S_F^{-1}, then the semi-boundedness of S_T is equivalent to the semi-boundedness of T.*

Proof. Since S_F^{-1} is compact, the spectrum of S_F only consists of a discrete set of eigenvalues, each of finite multiplicity, whence the bound (c) in the proof of Corollary 2.3.4 and the same conclusion as in Corollary 2.3.4(i). $\qquad\square$

Remark 2.3.6. The question of Theorem 2.3.3 and its corollaries deal with is sometimes referred to as the *"semi-boundedness problem"*, that is, the problem of finding conditions under which the semi-boundedness of S_T and of T are equivalent (in general or under special circumstances). The fact that the compactness of S_F^{-1} is a sufficient condition (that is, Corollary 2.3.5) was noted originally by Grubb [59] and by Gorbačuk and Mihaĭlec [56] in the mid 1970's. More than a decade later the same property, and more generally the necessary and sufficient condition provided by Theorem 2.3.3, was proved *with a boundary triplets language* by Derkach and Malamud [37]. In fact, it is easy to recognise that the operator-valued function $\alpha \mapsto M(\alpha)$ defined in (2.3.1) is the Weyl function of a standard boundary triplet [104, Example 14.12]. In [37, Section 3] one can also find examples in which such a condition is violated. The conclusion of Corollary 2.3.4(ii) is easy to establish also with general Hilbert space and spectral arguments, with no reference to the KVB theory – see, e.g., [38, Lemma XIII.7.22] or [95, Theorem X.1, first corollary]).

Theorem 2.3.3 and (the proof of) Corollary 2.3.4 have a further noticeable consequence.

Corollary 2.3.7 ("Finite-dimensional" extensions are always semi-bounded)**.** *Given a semi-bounded and densely defined symmetric operator S on a Hilbert space $\mathcal{H}$, whose bottom is positive ($m(S) > 0$), all the self-adjoint extensions of S_T of S for which the parameter T, in the parametrisation (2.2.1) of Theorem 2.2.1, is a self-adjoint operator acting on a* finite-dimensional *subspace of $\ker S^*$ are semi-bounded. For the occurrence of unbounded below self-adjoint extensions it is necessary (not sufficient) that $\dim \overline{\mathcal{D}(T)} = \infty$.*

Proof. T is bounded (and hence also semi-bounded) because the Hilbert space $\overline{\mathcal{D}(T)}$ it acts on has finite dimension. Let $P_T : \mathcal{H} \to \mathcal{H}$ be the orthogonal projection onto $\overline{\mathcal{D}(T)}$ and set

$$\widetilde{M}(\alpha) \;:=\; P_T(\alpha\mathbb{1} + \alpha^2(S_F - \alpha\mathbb{1})^{-1})P_T \;=\; P_T\,M(\alpha)\,P_T\,, \qquad \alpha < m(S)\,.$$

One can repeat for $\widetilde{M}(\alpha)$ the same arguments used in the proof of Corollary 2.3.4 to establish the uniform divergence of $M(\alpha)$ to $-\infty$, thus obtaining the same property for $\widetilde{M}(\alpha)$ on the finite-dimensional space $\overline{\mathcal{D}(T)}$ (the assumption $\dim \overline{\mathcal{D}(T)} = d < +\infty$ implies $\dim E^{(S_F)}([0, 2R])\overline{\mathcal{D}(T)} =$

$d_R \leqslant d$, which is the analogue of formula (c) in the proof of Corollary 2.3.4, whence the same conclusion). Therefore $\exists\, \alpha < 0$, with $|\alpha|$ sufficiently large, such that

$$\alpha\|v\|^2 + \alpha^2 \langle v, (S_F - \alpha \mathbb{1})^{-1} v \rangle \;<\; m(T)\|v\|^2 \;\leqslant\; \langle v, Tv \rangle \qquad \forall v \in \mathcal{D}(T)\,,$$

which implies $m(S_T) > \alpha$ owing to (2.2.2). $\qquad\square$

Remark 2.3.8. It is also worth remarking that unless S is essentially self-adjoint, in all other cases (i.e., whenever $\dim \ker S^* \geqslant 1$) there is no *uniform* lower bound to the bottoms of the semi-bounded self-adjoint extensions of S. This is an immediate consequence of the bound $m(T) \geqslant m(S_T)$ given by (2.2.2) in Theorem 2.2.2, since it is enough to consider extension parameters $T = -\gamma\mathbb{1}$ for arbitrary $\gamma > 0$.

In the remaining part of this Section we turn to the negative spectrum of an extension S_T. It turns out that relevant properties of the negative discrete spectrum of S_T are controlled by the analogous properties for T. We cast in Theorem 2.3.9 and Corollary 2.3.10 below results that are found in Birman's original work [15] (formulated therein with the original parametrisation $S_B \leftrightarrow B$), apart from a number of ambiguities and redundancies that we have cleaned up.

For convenience let us define

$$\begin{aligned}
\sigma_-(S_T) &:= \sigma(S_T) \cap (-\infty, 0) \\
\sigma_-(T) &:= \sigma(T) \cap (-\infty, 0)\,.
\end{aligned} \tag{2.3.3}$$

Theorem 2.3.9 (Negative spectrum). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$) and let S_T be a generic self-adjoint extension of S according to the parametrisation (2.2.1) of Theorem 2.2.1. Then $\sigma_-(S_T)$ consists of a bounded below set of finite-rank eigenvalues of S_T whose only possible accumulation point is 0 if and only if $\sigma_-(T)$ has the same property. When this is the case, and $\lambda_1 \leqslant \lambda_2 \leqslant \cdots < 0$ and $t_1 \leqslant t_2 \leqslant \cdots < 0$ are the ordered sequences of negative eigenvalues (counted with multiplicity) of S_T and of T respectively, then*

- *ground state of $S_T = \lambda_1 \leqslant t_1 =$ ground state of T,*

- *$\lambda_k \leqslant t_k$ for $k = 1, 2, \ldots$*

Corollary 2.3.10. *For some $N \in \mathbb{N}$, $\sigma_-(S_T)$ consists of N eigenvalues if and only if $\sigma_-(T)$ consists of N eigenvalues. (Here the eigenvalues are counted with multiplicity.)*

Remark 2.3.11. We observe that no restriction is assumed on the dimension of $\ker S^*$, that is, the deficiency index of S can be infinite as well. In fact, as long as $\dim \ker S^* < +\infty$, Corollary 2.3.10 could be deduced directly by combining Theorems 19 and 20 of Kreĭn's original work [74] with the subsequent results of Višik and Birman that are stated here in Theorems 2.2.1 and 2.2.3.

A further consequence is the following.

Corollary 2.3.12.

(i) *If S has finite deficiency index ($\dim \ker S^* < +\infty$), then all self-adjoint extensions of S have finite negative spectrum, with finite-dimensional eigenvalues.*

(ii) *If, in the sense of the parametrisation (2.2.1) of Theorem 2.2.1, S_T is a self-adjoint extension of S where the parameter T acts on a finite-dimensional subspace of $\ker S^*$, then the negative spectrum $\sigma_-(S_T)$ of S_T is finite, with finite-dimensional eigenvalues.*

In preparation for the proof of Theorem 2.3.9 and its corollaries, let us denote by $dE^{(S_T)}$ and by $dE^{(T)}$, respectively, the spectral measure of S_T and of T on $\mathbb{R}$. For generic $v \in \mathcal{D}(T)$ one also has $v \in \mathcal{D}[S_T]$ with $\langle v, Tv \rangle = S_T[v]$, owing to (2.2.6), whence

$$\int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle \;=\; \int_{[m(S_T), +\infty)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle \;\geqslant\; \int_{[m(S_T), 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle. \qquad (2.3.4)$$

Let us also single out two useful facts (the first is straightforward).

Lemma 2.3.13. *If V and W are closed subspaces of $\mathcal{H}$ with $\dim V < +\infty$ and $\dim W > \dim V$, then $W \cap V^\perp \neq \{0\}$.*

Lemma 2.3.14. *If $\varepsilon > 0$ and, for some $N \in \mathbb{N}$, $g_1, \ldots, g_N$ are linearly independent elements in $\mathcal{D}(S_T) \cap E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$, then the corresponding $v_1, \ldots, v_N$ given by the decomposition (2.2.1) $g_k = f_k + S_F^{-1}(Tv_k + w_k) + v_k$, $k = 1, \ldots, N$, are linearly independent in $\mathcal{D}(T)$.*

Proof. If $\sum_{k=1}^N c_k v_k = 0$ for some $c_1, \ldots, c_N \in \mathbb{C}$, then $g := \sum_{k=1}^N c_k g_k = \sum_{k=1}^N c_k (f_k + S_F^{-1}(Tv_k + w_k)) \in \mathcal{D}(S_F)$, whence $\langle g, S_T g \rangle = \langle g, S_F g \rangle \geqslant m(S)\|g\|^2 \geqslant 0$. On the other hand,

$$\langle g, S_T g \rangle \;=\; \int_{[m(S_T), +\infty)} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle \;=\; \int_{[m(S_T), -\varepsilon]} \lambda \langle g, dE^{(S_T)}(\lambda)g \rangle$$
$$\leqslant\; -\varepsilon \int_{[m(S_T), -\varepsilon]} \langle g, dE^{(S_T)}(\lambda)g \rangle \;\leqslant\; 0$$

(where in the second identity we used that $g \in \mathcal{D}(S_T) \cap E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$), therefore $g = 0$ and hence, by assumption, $c_1 = \cdots = c_N = 0$. $\qquad\qquad\square$

Proof of Theorem 2.3.9. Assume that $\sigma_-(S_T)$ consists of a bounded below set of finite-rank eigenvalues of S_T whose only possible accumulation point is 0. In particular, $-\infty < m(S_T) < 0$ which, by (2.2.2)-(2.2.3), implies also $m(S_T) \leqslant m(T) < 0$. If, for contradiction, $\sigma_-(T)$ does not satisfy the same property of $\sigma_-(S_T)$, then there exists $\varepsilon > 0$ such that $\dim E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)} = +\infty$, whereas by assumption $\dim E^{(S_T)}([m(S_T), -\frac{1}{2}\varepsilon])\mathcal{H} < +\infty$. By Lemma 2.3.13 $\exists v \in E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)}$, $v \neq 0$, $v \perp E^{(S_T)}([m(S_T), -\frac{1}{2}\varepsilon])\mathcal{H}$. As a consequence of this and of (2.3.4),

$$-\varepsilon\|v\|^2 \;\geqslant\; \int_{[m(T), -\varepsilon]} t \langle v, dE^{(T)}(t)v \rangle \;=\; \int_{[m(T), +\infty)} t \langle v, dE^{(T)}(t)v \rangle$$
$$\geqslant\; \int_{[m(S_T), 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle \;=\; \int_{(-\frac{1}{2}\varepsilon, 0)} \lambda \langle v, dE^{(S_T)}(\lambda)v \rangle \;\geqslant\; -\frac{\varepsilon}{2}\|v\|^2,$$

which is a contradiction because $v \neq 0$. For the converse, assume that $\sigma_-(T)$ consists of a bounded below set of finite-rank eigenvalues of T whose only possible accumulation point is 0. In particular, $-\infty < m(T) < 0$. If, for contradiction, $\sigma_-(S_T)$ does not satisfy the same property of $\sigma_-(T)$, then $\dim E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} = +\infty$ for some $\varepsilon > 0$. Therefore also

$$\dim E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T) \;=\; +\infty \qquad\qquad (*)$$

because $E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$ is dense in $E^{(S_T)}((-\infty, -\varepsilon])\mathcal{H}$. Based on the decomposition (2.2.1) for generic $g \in \mathcal{D}(S_T)$ (namely, $g = f + S_F^{-1}(Tv + w) + v$), set

$$V_\varepsilon \;:=\; \left\{ v \in \mathcal{D}(T) \,\middle|\, \begin{array}{l} g - v \in \mathcal{D}(S_F) \text{ for some} \\ g \in E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T) \end{array} \right\}.$$

In fact, owing to Lemma 2.3.14, any $v \in V_\varepsilon$ identifies uniquely the corresponding $g \in E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$. Furthermore, Lemma 2.3.14 and (*) yield $\dim V_\varepsilon = +\infty$. On the other hand, let $h \in \mathbb{R}$ with $0 < h < \min\{-m(T), \frac{\varepsilon m(S)}{2m(S)+\varepsilon}\}$: by assumption

$$\dim E^{(T)}([m(T), -h])\overline{\mathcal{D}(T)} \; < \; +\infty. \tag{**}$$

Lemma 2.3.13 and (*)-(**) then imply the existence of a non-zero $v \in V_\varepsilon$ with $v \perp E^{(T)}([m(T), -h])\overline{\mathcal{D}(T)}$. For such v one has

$$\langle v, Tv \rangle \; = \; \int_{[m(T), +\infty)} t \, \langle v, dE^{(T)}(t)v \rangle \; = \; \int_{(-h, +\infty)} t \, \langle v, dE^{(T)}(t)v \rangle \; \geqslant \; -h\|v\|^2$$
$$\geqslant \; -\frac{\varepsilon m(S)}{2m(S)+\varepsilon}\|v\|^2$$

which can be re-written equivalently as

$$\langle v, Tv \rangle + \frac{\varepsilon}{2}\|v\|^2 \; \geqslant \; \frac{\varepsilon^2}{4} \frac{1}{m(S) + \frac{1}{2}\varepsilon}\|v\|^2 \,.$$

The last inequality implies

$$\langle v, Tv \rangle + \frac{\varepsilon}{2}\|v\|^2 \; \geqslant \; \frac{\varepsilon^2}{4}\langle v, (S_F + \tfrac{1}{2}\varepsilon)^{-1}v \rangle \,.$$

If g is the vector in $E^{(S_T)}(-\infty, -\varepsilon])\mathcal{H} \cap \mathcal{D}(S_T)$ that corresponds to such $v \in V_\varepsilon$, by repeating the very same reasoning as in the proof of [51, Theorem 2.15] one sees that the latter condition is *equivalent* to $\langle g, S_T g \rangle \geqslant -\frac{\varepsilon}{2}\|g\|^2$. However, this last finding is not compatible with the fact that

$$\langle g, S_T g \rangle \; = \; \int_{[m(S_T), +\infty)} \lambda \, \langle g, dE^{(S_T)}(\lambda)g \rangle \; = \; \int_{[m(S_T), -\varepsilon]} \lambda \, \langle g, dE^{(S_T)}(\lambda)g \rangle \; \leqslant \; -\varepsilon\|g\|^2 \,,$$

whence the contradiction. This completes the proof of the equivalence of the considered condition for $\sigma_-(S_T)$ and $\sigma_-(T)$. When such a condition holds and the eigenvalues are labelled as in the statement of the theorem, obviously $\lambda_1 = m(S_T) \leqslant m(T) = t_1$ (by (2.2.2)), while the fact that $\lambda_k \leqslant t_k$ for $k = 1, 2, \ldots$ is a consequence of the min-max principle for the self-adjoint operators S_T and T, owing to the fact (Theorem 2.2.3) that $S_T \leqslant T$. $\qquad\square$

Proof of Corollary 2.3.10. Owing to Theorem 2.3.9,

$$\sigma_-(S_T) = \{\text{eigenvalues } \lambda_1 \leqslant \cdots \leqslant \lambda_N < 0\} \qquad \text{for some } N \in \mathbb{N}$$

is equivalent to

$$\sigma_-(T) = \{\text{eigenvalues } t_1 \leqslant \cdots \leqslant t_M < 0\} \qquad \text{for some } M \in \mathbb{N}$$

and when this is the case $\lambda_1 = m(S_T) \leqslant m(T) = t_1$. If $M > N$, then $\exists v \in (E^{(T)}([m(T), -\varepsilon])\overline{\mathcal{D}(T)}) \cap (E^{(S_T)}([m(S_T), 0))\mathcal{H})^\perp$, $v \neq 0$, for some $\varepsilon > 0$ (in fact, $\forall \varepsilon \in (0, |t_M|)$), as a consequence of Lemma 2.3.13. Moreover, $v \in \mathcal{D}(T)$ because

$$\int_{[m(T), +\infty)} t^2 \langle v, dE^{(T)}(t)v \rangle \; = \; \int_{[m(T), -\varepsilon]} t^2 \langle v, dE^{(T)}(t)v \rangle \; < \; +\infty \,,$$

whence also $v \in \mathcal{D}[S_T]$ with $S_T[v] = \langle v, Tv \rangle$, owing to (2.2.6). As a consequence of this and of (2.3.4),

$$0 > \int\limits_{[m(T), -\varepsilon]} t \langle v, \mathrm{d}E^{(T)}(t)v \rangle = \int\limits_{[m(T), +\infty)} t \langle v, \mathrm{d}E^{(T)}(t)v \rangle \geqslant \int\limits_{[m(S_T), 0)} \lambda \langle v, \mathrm{d}E^{(S_T)}(\lambda)v \rangle = 0,$$

a contradiction. If instead $M < N$, let us use the fact that for some $\varepsilon > 0$ (in fact $\forall \varepsilon \in (0, |\lambda_N|)$) Lemma 2.3.14 applied to the space V_ε introduced in the proof of Theorem 2.3.9 yields $\dim V_\varepsilon \geqslant N$: then, owing to Lemma 2.3.13, $\exists v \in V_\varepsilon \cap (E^{(T)}([m(T), 0))\overline{\mathcal{D}(T)})^\perp$, $v \neq 0$. In turn, as already observed in the proof of Theorem 2.3.9, this v identifies uniquely a non-zero element $g \in E^{(S_T)}([m(S_T), -\varepsilon])\mathcal{H} \subset \mathcal{D}(S_T)$ for which $g - v \in \mathcal{D}(S_F)$. For such g and v, (2.2.6) yields $\langle g, S_T g \rangle \geqslant \langle v, Tv \rangle$. With these findings,

$$
\begin{aligned}
0 &> \int\limits_{[m(S_T), -\varepsilon]} \lambda \langle g, \mathrm{d}E^{(S_T)}(\lambda)g \rangle = \int\limits_{[m(S_T), +\infty)} \lambda \langle g, \mathrm{d}E^{(S_T)}(\lambda)g \rangle = \langle g, S_T g \rangle \\
&\geqslant \langle v, Tv \rangle = \int\limits_{[m(T), +\infty)} t \langle v, \mathrm{d}E^{(T)}(t)v \rangle \geqslant \int\limits_{[m(T), 0)} t \langle v, \mathrm{d}E^{(T)}(t)v \rangle = 0,
\end{aligned}
$$

another contradiction. Thus, the conclusion is necessarily $M = N$. $\square$

Proof of Corollary 2.3.12. In either case (i) and (ii) the extension parameter T is self-adjoint on a finite-dimensional space, therefore its spectrum only consists of a finite number of (finite-dimensional) eigenvalues. This is true in particular for the negative spectrum of T. Then the conclusion follows from Corollary 2.3.10. $\square$

2.4   Resolvents of self-adjoint extensions

We turn now to the discussion of the structure of the resolvent of self-adjoint extensions.

In fact, this is a context in which the theory of boundary triplets (the modern theory that has "incorporated" the original KVB results, as it is briefly discussed in the Introduction) has deepest results, including the appropriate abstract language to reproduce in full generality the celebrated Kreĭn-Naimark resolvent formula – see, e.g., the comprehensive overview in [104, Chapter 14]. Here we content ourselves to discuss some direct applications of the KVB theory. We thus derive the formula of the inverse of an invertible extension *in terms of its KVB extension parameter* and of the "canonical" Friedrichs extension (Theorem 2.4.1), and from it we derive resolvent formulas (Corollary 2.4.2 and Theorem 2.4.4) originally established, in implicit form, by Kreĭn [74, Theorem 20].

Theorem 2.4.1 (Resolvent formula for invertible extensions)**.** *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$). Let, in terms of the decomposition and parametrisation (2.2.1) of Theorem 2.2.1, S_T be a generic self-adjoint extension of S and $P_T : \mathcal{H} \to \mathcal{H}$ be the orthogonal projection onto $\overline{\mathcal{D}(T)}$. If S_T is invertible on the whole $\mathcal{H}$, then T is invertible on the whole $\overline{\mathcal{D}(T)}$ and*

$$S_T^{-1} = S_F^{-1} + P_T T^{-1} P_T. \tag{2.4.1}$$

Proof. The invertibility (with everywhere defined inverse) of T is guaranteed by Theorem 2.3.1(iii). Thus, (2.4.1) is an identity between bounded self-adjoint operators (their boundedness following by the inverse mapping theorem). For a generic $h \in \mathcal{H} = \operatorname{ran} S_T$ one has $h = S_T g$ for some $g = f + S_F^{-1}(Tv + w) + v = F + v$, where $f \in \mathcal{D}(\overline{S})$, $v \in \mathcal{D}(T)$, $w = \ker S^* \cap \mathcal{D}(T)$ (Theorem 2.2.1), and hence $F \in \mathcal{D}(S_F)$ (Remark 2.1.3). Then

$$\langle h, S_T^{-1} h \rangle = \langle g, S_T g \rangle = \langle F, S_F F \rangle + \langle v, Tv \rangle.$$

On the other hand

$$\langle F, S_F F \rangle \;=\; \langle S_F F, S_F^{-1} S_F F \rangle \;=\; \langle S_T g, S_F^{-1} S_T g \rangle \;=\; \langle h, S_F^{-1} h \rangle$$

and

$$\langle v, T v \rangle \;=\; \langle T v, T^{-1} T v \rangle \;=\; \langle P_T S_T g, T^{-1} P_T S_T g \rangle \;=\; \langle h, P_T T^{-1} P_T h \rangle \,,$$

whence the conclusion $\langle h, S_T^{-1} h \rangle = \langle h, S_F^{-1} h \rangle + \langle h, P_T T^{-1} P_T h \rangle$. $\qquad\square$

Corollary 2.4.2. *Let $\widetilde{S}$ be a self-adjoint extension of S and let $z < m(S)$ be such that $\widetilde{S} - z\mathbb{1}$ is invertible on the whole $\mathcal{H}$ (for example a semi-bounded extension $\widetilde{S}$ and a real number $z < m(\widetilde{S})$). Let $T(z)$ be the extension parameter, in the sense of the KVB parametrisation (2.2.1) of Theorem 2.2.1, of the operator $\widetilde{S} - z\mathbb{1}$ considered as a self-adjoint extension of the densely defined and bottom-positive symmetric operator $S(z) := S - z\mathbb{1}$. Correspondingly, let $P(z)$ be the orthogonal projection onto $\overline{\mathcal{D}(T(z))}$. Then*

$$(\widetilde{S} - z\mathbb{1})^{-1} \;=\; (S_F - z\mathbb{1})^{-1} + P(z)\, T(z)^{-1} P(z) \,. \tag{2.4.2}$$

Proof. Since $m(S(z)) = m(S) - z > 0$, the assumptions of Theorem 2.4.1 are matched and (2.4.1) takes the form (2.4.2) owing to the fact that the Friedrichs extension of $S(z)$ is precisely $S_F - z\mathbb{1}$ (Theorem 1.3.2(vii)). $\qquad\square$

Remark 2.4.3. Formula (2.4.2), in particular, shows that the resolvent difference $(\widetilde{S} - z\mathbb{1})^{-1} - (S_F - z\mathbb{1})^{-1}$ has non-zero matrix elements only on a suitable subspace of $\ker(S^* - z\mathbb{1})$. (The dependence on z of the term $P(z)T(z)^{-1}P(z)$ remains here somewhat implicit, although of course $T(z)$ and $P(z)$ are unambiguously and constructively well defined in terms of the given $\widetilde{S} - z\mathbb{1}$, as described in Proposition 2.2.6.)

Let us now make (2.4.2) more explicit by reproducing a Kreĭn-like resolvent formula (see, e.g., [4, Theorems A.2-A.3]).

Theorem 2.4.4 (Kreĭn's resolvent formula for deficiency index = 1)**.** *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ with positive bottom ($m(S) > 0$) and with deficiency index $\dim \ker S^* = 1$. Let $\widetilde{S}$ be a self-adjoint extension of S other than the Friedrichs extension S_F. Let $v \in \ker S^* \setminus \{0\}$ and for each $z \in (-\infty, m(S)) \cap \rho(\widetilde{S})$ set*

$$v(z) \;:=\; v + z(S_F - z\mathbb{1})^{-1} v \,. \tag{2.4.3}$$

Then there exists an analytic function $\beta : (-\infty, m(S)) \cap \rho(\widetilde{S}) \to \mathbb{R}$, with $\beta(z) \neq 0$, such that

$$(\widetilde{S} - z\mathbb{1})^{-1} \;=\; (S_F - z\mathbb{1})^{-1} + \beta(z)\, |v(z)\rangle\langle v(z)| \,. \tag{2.4.4}$$

$\beta(z)$, $v(z)$, and (2.4.4) admit an analytic continuation to $\rho(S_F) \cap \rho(\widetilde{S})$.

Proof. Because of the constance of the deficiency index, $\dim \ker(S^* - z\mathbb{1}) = \dim \ker S^* = 1$. $\widetilde{S}$ is semi-bounded (Corollary 2.3.4). Since $z < m(\widetilde{S})$, $\widetilde{S} - z\mathbb{1}$ is a bottom-positive self-adjoint extension of the densely defined and bottom-positive symmetric operator $S(z) := S - z\mathbb{1}$. Its extension parameter $T(z)$, in the sense of the KVB parametrisation, is the bottom-positive self-adjoint operator $T(z)$ on the space $\ker(S^* - z\mathbb{1})$ which acts as the multiplication by a positive number $t(z)$. (The positivity of the bottom of $T(z)$ follows from $m(T(z)) \geqslant m(\widetilde{S} - z\mathbb{1}) > 0$, Theorem 2.3.3.) Clearly, $v(z) \in \ker(S^* - z\mathbb{1})$. Moreover, $v(z) \neq 0$ for each admissible z: this is obviously true if $z = 0$, and if it was not true for $z \neq 0$, then $z(S_F - z\mathbb{1})^{-1} v = -v \neq 0$, which would contradict $\mathcal{D}(S_F - z\mathbb{1}) \cap \ker(S^* - z\mathbb{1}) = \{0\}$ (Remark 2.1.3, formula (2.1.7)). Thus, $v(z)$ spans $\ker(S^* - z\mathbb{1})$ and $P_T := \|v(z)\|^{-2} |v(z)\rangle\langle v(z)| : \mathcal{H} \to \mathcal{H}$ is the orthogonal projection onto $\ker(S^* - z\mathbb{1})$. In this case, the resolvent formula (2.4.2) takes precisely the form (2.4.4) where $\beta(z) := \|v(z)\|^{-4} t(z)^{-1}$. Being a product of positive quantities,

$\beta(z) > 0$. Moreover, $z \mapsto (\widetilde{S} - z\mathbb{1})^{-1}$ and $z \mapsto (S_F - z\mathbb{1})^{-1}$ are analytic operator-valued functions on the whole $\rho(S_F) \cap \rho(\widetilde{S})$ (because of the analyticity of resolvents) and so is the vector-valued function $z \mapsto v(z)$ (because of the construction (2.4.3)). Therefore, taking the expectation of both sides of (2.4.4) on $v(z)$ shows at once that $z \mapsto \beta(z)$ is analytic on $\rho(S_F) \cap \rho(\widetilde{S})$, and real analytic on $(-\infty, m(S)) \cap \rho(\widetilde{S})$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

2.5 Examples

2.5.1 "Free quantum particle" on half-line

On the Hilbert space $\mathcal{H} = L^2[0, +\infty)$ one considers the densely defined symmetric operator

$$S = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}, \qquad \mathcal{D}(S) = C_0^\infty(0, +\infty). \tag{2.5.1}$$

S has bottom $m(S) = 1$. One has

$$S^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}$$

$$\mathcal{D}(S^*) = H^2(0, +\infty) = \left\{ f \in L^2[0 + \infty) \,\middle|\, \begin{matrix} f, f' \in AC[0, +\infty) \\ f'' \in L^2[0, +\infty) \end{matrix} \right\}, \tag{2.5.2}$$

thus all the extensions of S act as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}$ on suitable restrictions of $H^2(0, +\infty)$. In particular,

$$\mathcal{D}(\overline{S}) = H_0^2(0, +\infty) = \{ f \in H^2(0, +\infty) \,|\, f(0) = 0, \ f'(0) = 0 \} \tag{2.5.3}$$

and the Friedrichs extension of S has domain

$$\mathcal{D}(S_F) = H^2(0, +\infty) \cap H_0^1(0, +\infty) = \{ f \in H^2(0, +\infty) \,|\, f(0) = 0 \}, \tag{2.5.4}$$

that is, $\mathcal{D}(S^*)$ with Dirichlet boundary condition at the origin.

Applying von Neumann's theory one finds (see, e.g., [55, Chapter 6.2]) that the self-adjoint extensions of S constitute the family $\{ S_\nu \,|\, \nu \in (-\frac{\pi}{2}, \frac{\pi}{2}] \}$, where each S_ν acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}$ on the domain

$$\mathcal{D}(S_\nu) = \{ g \in H^2(0, +\infty) \,|\, g(0) \sin \nu = g'(0) \cos \nu \}. \tag{2.5.5}$$

By inspection one sees that the Friedrichs extension of S is $S_{\pi/2}$.

In order to apply the KVB theory, one needs to identify $\ker S^*$ and S_F^{-1}. One easily finds

$$\ker S^* = \mathrm{Span}\{ e^{-x} \}. \tag{2.5.6}$$

All self-adjoint extensions of S are therefore semi-bounded (Corollary 2.3.4). One also finds that the integral kernel of S_F^{-1} is

$$S_F^{-1}(x, y) = \frac{1}{2} \big(e^{-|x-y|} - e^{-(x+y)} \big) \tag{2.5.7}$$

(see, e.g., [55, Chapter 6.2]). In fact, since S_F^{-1} only enters the formulas as acting on $\ker S^*$, instead of (2.5.7) one can rather limit oneself to the problem

$$\begin{cases} -\eta''(x) + \eta(x) = e^{-x}, & x \in [0, +\infty) \\ \eta(0) = 0, \end{cases}$$

whose only solution in $L^2[0, +\infty)$ is $\eta(x) = \frac{1}{2} x\, e^{-x}$. Thus, for fixed $a \in \mathbb{C}$,

$$S_F^{-1}(a\, e^{-x}) \;=\; \frac{a}{2}\, x\, e^{-x}\,. \tag{2.5.8}$$

According to Theorem 2.2.1, the self-adjoint extensions of S are operators of the form S_T where T is a self-adjoint operator on subspaces of $\ker S^* = \mathrm{Span}\{e^{-x}\}$, precisely the zero-dimensional subspace $\{0\}$ or the whole $\mathrm{Span}\{e^{-x}\}$. In the former case $S_T = S_F$ (Proposition 2.2.4). In the latter, each such T acts as the multiplication $T_\beta : e^{-x} \mapsto \beta e^{-x}$ by a fixed $\beta \in \mathbb{R}$, $\mathcal{D}(T_\beta) = \mathrm{Span}\{e^{-x}\} = \ker S^*$, and $\ker S^* \cap \mathcal{D}(T_\beta)^\perp = \{0\}$: by (2.2.1) and (2.5.8), the corresponding self-adjoint extension $S_\beta \equiv S_{T_\beta}$ of S acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \mathbb{1}$ on the domain

$$
\begin{aligned}
\mathcal{D}(S_\beta) \;&=\; \left\{ g = f + S_F^{-1}(\beta\, a\, e^{-x}) + a\, e^{-x} \;\middle|\; \begin{array}{c} f \in H_0^2(0, +\infty) \\ a \in \mathbb{C} \end{array} \right\} \\
&=\; \left\{ g \;\middle|\; \begin{array}{c} g(x) = f(x) + a\left(\frac{1}{2}\beta x + 1\right) e^{-x} \\ x \in [0, 1]\,,\ f \in H_0^2(0, +\infty)\,,\ a \in \mathbb{C} \end{array} \right\}.
\end{aligned}
\tag{2.5.9}
$$

Observing that $g(0) = a$ and $g'(0) = a(\frac{1}{2}\beta - 1)$ for any $g \in \mathcal{D}(S_\beta)$, (2.5.9) can be re-written as

$$\mathcal{D}(S_\beta) \;=\; \left\{ g \in H^2(0, +\infty)\,\middle|\, g'(0) = \left(\frac{\beta}{2} - 1\right) g(0) \right\}. \tag{2.5.10}$$

Comparing (2.5.10) with (2.5.5) above, we see that S_β is the extension S_ν of von Neumann's parametrisation with

$$\beta/2 - 1 \;=\; \tan\nu \tag{2.5.11}$$

which includes the Friedrichs extension ($\nu = \frac{\pi}{2}$) if one let $\beta = +\infty$.

The same analysis can be equivalently performed in terms of the quadratic forms of the self-adjoint extensions of S, following Theorem 2.2.3 (which applies to this example since *all* extensions are semi-bounded). The reference form is the Friedrichs one, that is,

$$
\begin{aligned}
\mathcal{D}[S_F] \;&=\; H_0^1(0, +\infty) \;=\; \{f \in H^1[0, +\infty)\,|\, f(0) = 0\} \\
S_F[F_1, F_2] \;&=\; \int_0^{+\infty} \overline{F_1'(x)}\, F_2'(x)\, \mathrm{d}x + \int_0^{+\infty} \overline{F_1(x)}\, F_2(x)\, \mathrm{d}x\,,
\end{aligned}
\tag{2.5.12}
$$

as one deduces from (2.5.4). Owing to (2.2.6), the form domain of any other extension is obtained by taking the direct sum of $\mathcal{D}[S_T] = \mathcal{D}[S_F] \dotplus \mathcal{D}[T]$ where $T \equiv T_\beta =$ the multiplication by a real β on $\mathcal{D}(T) = \mathrm{Span}\{e^{-x}\} = \mathcal{D}[T]$. Then (2.2.6) and (2.5.12) yield

$$
\begin{aligned}
\mathcal{D}[S_\beta] \;&=\; H_0^1(0, +\infty) \dotplus \mathrm{Span}\{e^{-x}\} \;=\; H^1(0, +\infty) \\
S_\beta[g_1, g_2] \;&=\; S_\beta[F_1 + a_1\, e^{-x}, F_2 + a_2\, e^{-x}] \\
&=\; \int_0^{+\infty} \overline{F_1'(x)}\, F_2'(x)\mathrm{d}x + \int_0^{+\infty} \overline{F_1(x)}\, F_2(x)\, \mathrm{d}x + \frac{\beta}{2}\, \overline{a_1}\, a_2 \\
&=\; \int_0^{+\infty} \overline{g_1'(x)}\, g_2'(x)\mathrm{d}x + \int_0^{+\infty} \overline{g_1(x)}\, g_2(x)\, \mathrm{d}x + \left(\frac{\beta}{2} - 1\right) \overline{g_1(0)}\, g_2(0)\,.
\end{aligned}
\tag{2.5.13}
$$

Going backwards from this (closed and semi-bounded) form to the uniquely associated self-adjoint operator, a straightforward exercise would yield the domain $\mathcal{D}(S_\beta)$ already determined by (2.5.10).

Concerning the bottom and the negative spectrum of a generic extension S_β, one has $m(T_\beta) = \beta$ and $\sigma(T_\beta) = \{\beta\}$, therefore Theorem 2.2.2 gives

$$
\begin{aligned}
m(S_\beta) \;&\leqslant\; \min\{1, \beta\} \qquad \forall \beta \in \mathbb{R} \\
\frac{\beta}{1 + \beta} \;\leqslant\; m(S_\beta) \;&\leqslant\; \min\{1, \beta\} \qquad \text{if } \beta > -1
\end{aligned}
\tag{2.5.14}
$$

and Corollary 2.3.10 implies that $\sigma_-(S_\beta)$ consists of one single eigenvalue whenever $\beta < 0$. The explicit spectral analysis of S_β gives $\sigma_-(S_\beta) = \emptyset$ if $\beta \geqslant 2$ and $\sigma_-(S_\beta) = \{1 - (\beta/2 - 1)^2)\}$ if $\beta < 2$ with normalised eigenfunction $g_\beta(x) = \sqrt{2 - \beta}\, e^{-(1-\beta/2)x}$, whence

$$m(S_\beta) \; = \; \begin{cases} 1 & \beta \geqslant 2 \\ 1 - (\beta/2 - 1)^2 & \beta < 2\,. \end{cases} \tag{2.5.15}$$

We thus see that the bounds (2.5.14) are consistent with the "exact result" (2.5.15) (and that there are extensions other than the Friedrichs one whose bottom coincide with that of S).

As for the resolvents, for $z > 0$ one sees that $e^{-zx} \in \ker(S^* + (z^2 - 1)\mathbb{1})$ and by means of the formula ([55, Chapter 6.2])

$$(S_F + (z^2 - 1)\mathbb{1})^{-1}(x, y) \; = \; \frac{1}{2z}\big(e^{-z|x-y|} - e^{-z(x+y)}\big) \qquad (z > 0) \tag{2.5.16}$$

one finds

$$(S_\beta + (z^2 - 1)\mathbb{1})^{-1} \; = $$
$$= \; (S_F + (z^2 - 1)\mathbb{1})^{-1} + \frac{1}{(\beta/2 - 1) + z}|e^{-zx}\rangle\langle e^{-zx}|, \quad z > 0, \tag{2.5.17}$$

for $z > 0$ and $z \neq -(\beta/2 - 1)$ if $\beta < 2$. This is precisely a Kreĭn resolvent formula of the type (2.4.4). The corresponding integral kernel is

$$(S_\beta + (z^2 - 1)\mathbb{1})^{-1}(x, y) \; = \; \frac{1}{2z}\Big(e^{-z|x-y|} - \frac{\beta/2 - 1 - z}{\beta/2 - 1 + z}e^{-z(x+y)}\Big). \tag{2.5.18}$$

This expression can be continued analytically to complex z's as stated in general in Theorem 2.4.4, see (2.5.23) below.

The shift by a unit constant introduced in the definition (2.5.1) of S guarantees that S has positive bottom. After having determined with (2.5.12)-(2.5.13) the quadratic forms of a generic self-adjoint extension of S, one can remove the shift and deduce that the self-adjoint extensions of the operator $S' = -\frac{d^2}{dx^2}$, $\mathcal{D}(S') = C_0^\infty(0, +\infty)$, constitute the family $\{S'_\beta \,|\, \beta \in (-\infty, +\infty]\}$ where for each $\beta \in \mathbb{R}$ the element S'_β is the extension with quadratic form

$$\mathcal{D}[S'_\beta] \; = \; H^1(0, +\infty)$$
$$S'_\beta[g_1, g_2] \; = \; \int_0^{+\infty} \overline{g'_1(x)}\, g'_2(x)\mathrm{d}x + \Big(\frac{\beta}{2} - 1\Big)\overline{g_1(0)}\, g_2(0)\,, \tag{2.5.19}$$

and hence with

$$\mathcal{D}(S'_\beta) \; = \; \Big\{g \in H^2(0, +\infty) \,|\, g'(0) = \Big(\frac{\beta}{2} - 1\Big)g(0)\Big\}$$
$$S'_\beta g \; = \; -g''\,, \tag{2.5.20}$$

whereas for $\beta = \infty$ one has the Friedrichs extensions

$$\mathcal{D}[S'_F] \; = \; H_0^1(0, +\infty)\,, \qquad S'_\beta[g_1, g_2] \; = \; \int_0^{+\infty} \overline{g'_1(x)}\, g'_2(x)\mathrm{d}x\,,$$
$$\mathcal{D}(S'_F) \; = \; H^2(0, +\infty) \cap H_0^1(0, +\infty)\,, \qquad S'_F f = -f''\,. \tag{2.5.21}$$

Similarly, one deduces from (2.5.18)

$$(S'_\beta + z^2\mathbb{1})^{-1}(x, y) \; = \; \frac{1}{2z}\Big(e^{-z|x-y|} - \frac{\beta/2 - 1 - z}{\beta/2 - 1 + z}e^{-z(x+y)}\Big) \tag{2.5.22}$$

for $z > 0$ and $z \neq -(\beta/2 - 1)$ if $\beta < 2$. This expression admits the analytic continuation

$$(S'_\beta - k^2 \mathbb{1})^{-1}(x, y) \;=\; \frac{\mathrm{i}}{2k}\left(e^{\mathrm{i}k|x-y|} - \frac{(\beta/2 - 1) + \mathrm{i}k}{(\beta/2 - 1) - \mathrm{i}k}e^{\mathrm{i}k(x+y)}\right) \tag{2.5.23}$$

for $k \in \mathbb{C}$ with $\mathfrak{Im}\, k > 0$ and $k \neq -\mathrm{i}(\beta/2 - 1)$ if $\beta < 2$, that is, the operator-valued map $\mathbb{C} \ni k^2 \mapsto (S'_\beta - k^2 \mathbb{1})^{-1}$ is holomorphic.

2.5.2 "Free quantum particle" on an interval

On the Hilbert space $\mathcal{H} = L^2[0, 1]$ one considers the densely defined symmetric operator

$$S \;=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\,, \qquad\qquad \mathcal{D}(S) \;=\; C_0^\infty(0, 1)\,. \tag{2.5.24}$$

The positivity of the bottom of S can be seen by applying twice (to f, f' and to f', f'') Poincaré's inequality

$$\int_0^1 |f'(x)|^2 \mathrm{d}x \;\geqslant\; \pi^2 \int_0^1 |f(x)|^2 \mathrm{d}x \qquad \forall f \in C_0^\infty(0, 1)\,,$$

thus obtaining

$$m(S) \;=\; \pi^2\,. \tag{2.5.25}$$

One has

$$S^* \;=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$
$$\mathcal{D}(S^*) \;=\; H^2(0, 1) = \left\{ f \in L^2[0, 1] \,\middle|\, \begin{matrix} f, f' \in AC[0, 1] \\ f'' \in L^2[0, 1] \end{matrix} \right\}, \tag{2.5.26}$$

thus all the extensions of S act as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on suitable restrictions of $H^2(0, 1)$. In particular,

$$\mathcal{D}(\overline{S}) \;=\; H_0^2(0, 1) \;=\; \left\{ f \in H^2(0, 1) \,\middle|\, \begin{matrix} f(0) = 0 = f(1) \\ f'(0) = 0 = f'(1) \end{matrix} \right\} \tag{2.5.27}$$

and the Friedrichs extension of S has domain

$$\mathcal{D}(S_F) \;=\; H^2(0, 1) \cap H_0^1(0, 1) \;=\; \{ f \in H^2(0, 1) \,|\, f(0) = 0 = f(1) \}\,, \tag{2.5.28}$$

that is, S_F is the negative Laplacian with Dirichlet boundary conditions. Considering its spectrum, $\sigma(S_F) = \{ n^2\pi^2 \,|\, n \in \mathbb{N} \}$, one re-obtains (2.5.25) without using Poincaré's inequality.

Applying von Neumann's theory one finds (see, e.g., [55, Chapter 6.2]) that the self-adjoint extensions of S constitute the family $\{ S_U \,|\, U \in U(2) \}$ where each S_U acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on the domain

$$\mathcal{D}(S_U) \;=\; \left\{ g \in H^2(0, 1) \,\middle|\, \begin{pmatrix} g(1) - \mathrm{i}g'(1) \\ g(0) + \mathrm{i}g'(0) \end{pmatrix} = U \begin{pmatrix} g(1) + \mathrm{i}g'(1) \\ g(0) - \mathrm{i}g'(0) \end{pmatrix} \right\}. \tag{2.5.29}$$

By inspection one sees that in this case the Friedrichs extension of S is the extension S_U indexed by $U = -\mathbb{1}$.

Let us apply now the KVB theory, identifying first of all $\ker S^*$ and S_F^{-1}. One has

$$\ker S^* \;=\; \mathrm{Span}\{ \mathbf{1}, x \}\,. \tag{2.5.30}$$

All self-adjoint extensions of S are therefore semi-bounded (Corollary 2.3.4). As for S_F^{-1}, all what we need here is its action on $\ker S^*$ (the general inversion formula for the problem $S_F \eta = h$ with datum h can be found, for instance, in [55, Chapter 6.2]), therefore we consider the problem

$$\begin{cases} -\eta''(x) = a + bx\,, & x \in [0,1] \\ \eta(0) = 0 = \eta(1) \end{cases}$$

for given $a, b \in \mathbb{C}$, whose only solution is $\eta(x) = (\frac{a}{2} + \frac{b}{6})x - \frac{a}{2}x^2 - \frac{b}{6}x^3$. Thus,

$$S_F^{-1}(a + bx) \;=\; \left(\frac{a}{2} + \frac{b}{6}\right)x - \frac{a}{2}x^2 - \frac{b}{6}x^3\,, \qquad x \in [0,1]\,. \tag{2.5.31}$$

Owing to (2.5.27), (2.5.30), and (2.5.31) above, the decomposition (2.1.6) reads

$$H^2(0,1) \cap H_0^1(0,1) \;=\; H_0^2(0,1) \,\dot{+}\, S_F^{-1}\mathrm{Span}\{\mathbf{1}, x\}$$

i.e., any $F \in H^2(0,1) \cap H_0^1(0,1)$ determines uniquely $f \in H_0^2(0,1)$ and $a, b \in \mathbb{C}$ such that $F(x) = f(x) + (\frac{a}{2} + \frac{b}{6})x - \frac{a}{2}x^2 - \frac{b}{6}x^3$. Explicitly,

$$F(x) \;=\; f(x) + F'(0)x - (2F'(0) + F'(1))x^2 + (F'(0) + F'(1))x^3\,.$$

Analogously, the decomposition (2.1.4) reads

$$H^2(0,1) \;=\; H^2(0,1) \cap H_0^1(0,1) + \mathrm{Span}\{\mathbf{1}, x\}\,,$$

that is, any $g \in H^2(0,1)$ can be written as

$$g(x) \;=\; F(x) + g(0) + (g(1) - g(0))x$$

for a unique $F \in H^2(0,1) \cap H_0^1(0,1)$.

According to Theorem 2.2.1, the self-adjoint extensions of S are operators of the form S_T where T is a self-adjoint operator on subspaces of $\ker S^* = \mathrm{Span}\{\mathbf{1}, x\}$, precisely

- the zero-dimensional subspace $\{0\}$, in which case $S_T = S_F$ (Proposition 2.2.4)

- or the one-dimensional subspaces $\mathrm{Span}\{\mathbf{1}\}$ or $\mathrm{Span}\{a\mathbf{1} + x\}$, $a \in \mathbb{C}$, in which case T acts as the multiplication by a real number,

- or the whole two-dimensional space $\mathrm{Span}\{\mathbf{1}, x\} \cong \mathbb{C}^2$, in which case T acts as the multiplication by a hermitian matrix.

For concreteness, let us work out in detail the case of the one-dimensional space $\mathrm{Span}\{\mathbf{1}\}$ and of the self-adjoint operator T_β on it, defined by $T_\beta \mathbf{1} := \beta \mathbf{1}$ for fixed $\beta \in \mathbb{R}$. In this case $\mathcal{D}(T_\beta) = \mathrm{Span}\{\mathbf{1}\}$ and $\ker S^* \cap \mathcal{D}(T_\beta)^\perp = \mathrm{Span}\{2x - \mathbf{1}\}$: therefore, according to (2.2.1), the corresponding self-adjoint extension $S_\beta \equiv S_{T_\beta}$ of S acts as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on the domain

$$\mathcal{D}(S_\beta) \;=\; \left\{ g = f + S_F^{-1}(\beta\gamma\mathbf{1} + \delta(2x - \mathbf{1})) + \gamma\mathbf{1} \,\middle|\, \begin{array}{l} f \in H_0^2(0,1) \\ \gamma, \delta \in \mathbb{C} \end{array} \right\}\,.$$

By means of (2.5.31) (upon renaming the coefficients γ, δ), this is re-written as

$$\mathcal{D}(S_\beta) \;=\; \left\{ g \,\middle|\, \begin{array}{l} g(x) = f(x) + 2\gamma + (\beta\gamma - \delta)x - (\beta\gamma - 3\delta)x^2 - 2\delta x^3 \\ x \in [0,1]\,, \quad f \in H_0^2(0,1)\,, \quad \gamma, \delta \in \mathbb{C} \end{array} \right\} \tag{2.5.32}$$

which in turn, observing that $g(0) = 2\gamma = g(1)$ and $g'(0) - g'(1) = 2\beta\gamma$ for any $g \in \mathcal{D}(S_\beta)$, can be further re-written as

$$\mathcal{D}(S_\beta) = \left\{ g \in H^2(0,1) \,\middle|\, \begin{array}{c} g(0) = g(1) \\ g'(0) - g'(1) = \beta g(0) \end{array} \right\}. \tag{2.5.33}$$

The special case $\beta = 0$ corresponds to the self-adjoint extension with periodic boundary conditions: in the parametrisation (2.5.29) of von Neumann's theory, this is the extension S_U with $U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Concerning the bottom of the extensions of the form S_β, clearly $m(T_\beta) = \beta$, thus Theorem 2.2.2 gives

$$\begin{aligned} m(S_\beta) &\leqslant \min\{\pi^2, \beta\} && \forall \beta \in \mathbb{R} \\ \frac{\beta\pi^2}{\beta + \pi^2} &\leqslant m(S_\beta) \leqslant \min\{\pi^2, \beta\} && \text{if } \beta > -\pi^2 \,. \end{aligned} \tag{2.5.34}$$

This is consistent with the explicit knowledge of $\sigma(S_\beta)$: for example $\sigma(S_{\beta=0}) = \{4\pi^2 n^2 \,|\, n \in \mathbb{Z}\}$, whence indeed $m(S_{\beta=0}) = 0$. Moreover, since $\sigma(T_\beta) = \{\beta\}$ (simple eigenvalue), Corollary 2.3.10 implies that $\sigma_-(S_\beta)$ consists of one single eigenvalue whenever $\beta < 0$.

All other cases of the above list can be discussed analogously: along the same line, (2.2.1) and (2.5.31) produce each time an expression like (2.5.32) for $\mathcal{D}(S_T)$ that can be then cast in the form (2.5.33). For completeness, we give here the summary of all possible conditions of self-adjointness. The family of all self-adjoint extension of S is described by the following four families of boundary conditions:

$$g'(0) = b_1 g(0) + cg(1)\,, \qquad g'(1) = -\bar{c}g(0) - b_2 g(1)\,, \tag{2.5.35}$$

$$g'(0) = b_1 g(0) + \bar{c}g'(1)\,, \qquad g(1) = cg(0)\,, \tag{2.5.36}$$

$$g'(1) = -b_1 g(1)\,, \qquad g(0) = 0\,, \tag{2.5.37}$$

$$g(0) = 0 = g(1)\,, \tag{2.5.38}$$

where $c \in \mathbb{C}$ and $b_1, b_2 \in \mathbb{R}$ are arbitrary parameters. For each boundary condition, the corresponding extension is the operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ acting on the $H^2(0,1)$-functions that satisfy that one boundary condition. For instance, the extension S_β determined by (2.5.33) correspond to the boundary condition of type (2.5.36) with $c = 1$ and $b_1 = \beta$. In term of the Višik-Birman extension parameter T, conditions of type (2.5.35) occur when $\dim \mathcal{D}(T) = 2$, conditions of type (2.5.36) or (2.5.37) occur when $\dim \mathcal{D}(T) = 1$, and condition (2.5.38) is precisely that occurring when $\dim \mathcal{D}(T) = 0$ (Dirichlet boundary conditions, Friedrichs extension). The well-known conditions (2.5.35)-(2.5.38) can be also found by means of boundary triplet techniques: see, e.g., [104, Example 4.10].

The same analysis can be equivalently performed in terms of the quadratic forms of the self-adjoint extensions of S, according to Theorem 2.2.3 (in the present case *all* extensions are semi-bounded). The reference form is the Friedrichs one, that is,

$$\begin{aligned} \mathcal{D}[S_F] &= H_0^1(0,1) = \left\{ f \in L^2[0,1] \,\middle|\, \begin{array}{c} f \in AC[0,1],\ f' \in L^2[0,1], \\ f(0) = 0 = f(1) \end{array} \right\} \\ S_F[F_1, F_2] &= \int_0^1 \overline{F_1'(x)}\, F_2'(x)\, \mathrm{d}x \qquad \forall F_1, F_2 \in \mathcal{D}[S_F]\,, \end{aligned} \tag{2.5.39}$$

as one deduces from (2.5.28). The property $m(S_F) = \pi^2$ reads

$$\int_0^1 |f'(x)|^2 \mathrm{d}x \;\geqslant\; \pi^2 \int_0^1 |f(x)|^2 \mathrm{d}x \qquad \forall f \in H_0^1(0,1)\,, \tag{2.5.40}$$

that is, Poincaré's inequality. Owing to (2.2.6), the form domain of each extension is obtained by taking the direct sum of $\mathcal{D}[S_T] = \mathcal{D}[S_F] \dotplus \mathcal{D}[T]$: in the present case $\mathcal{D}[T] = \mathcal{D}(T)$, because of the finiteness of the deficiency index of S. For example, in the concrete case worked out above, that is, $T \equiv T_\beta = $ multiplication by a real β on $\mathcal{D}(T) = \mathrm{Span}\{\mathbf{1}\}$, (2.2.6) and (2.5.39) yield

$$
\begin{aligned}
\mathcal{D}[S_\beta] &= H_0^1(0,1) \dotplus \mathrm{Span}\{\mathbf{1}\} = \{g \in H^1(0,1) \,|\, g(0) = g(1)\} \\
S_\beta[g_1, g_2] &= S_\beta[F_1 + \gamma_1 \mathbf{1}, F_2 + \gamma_2 \mathbf{1}] = \int_0^1 \overline{F_1'(x)}\, F_2'(x)\mathrm{d}x + \beta\,\overline{\gamma_1}\,\gamma_2 \\
&= \int_0^1 \overline{g_1'(x)}\, g_2'(x)\mathrm{d}x + \beta\overline{g_1(0)}\, g_2(0)\,.
\end{aligned}
\tag{2.5.41}
$$

Then, going from this (closed and semi-bounded) form to the uniquely associated self-adjoint operator, a straightforward exercise would yield the domain $\mathcal{D}(S_\beta)$ already determined by (2.5.33).

As for the Kreĭn-von Neumann extension S_N of S, this is the extension S_T with $T : \ker S^* \to \ker S^*$, $Tv = 0 \; \forall v \in \ker S^*$ (Proposition 2.2.4), in which case (2.2.6) and (2.5.39) yield the quadratic form

$$
\begin{aligned}
\mathcal{D}[S_N] &= H_0^1(0,1) \dotplus \mathrm{Span}\{\mathbf{1}, x\} = H^1(0,1) \\
S_N[g_1, g_2] &= S_N[F_1 + a_1\mathbf{1} + b_1 x, F_2 + a_2\mathbf{1} + b_2 x] \\
&= \int_0^1 \overline{F_1'(x)}\, F_2'(x)\, \mathrm{d}x \\
&= \int_0^1 \overline{g_1'(x)}\, g_2'(x)\, \mathrm{d}x - (\overline{g_1}(1) - \overline{g_1}(0))(g_2(1) - g_2(0))\,.
\end{aligned}
\tag{2.5.42}
$$

The corresponding S_N is either found by determining the self-adjoint operator associated to $S_N[\cdot]$ or by applying directly (2.2.1) to the operator T under consideration:

$$
\begin{aligned}
\mathcal{D}(S_N) &= H_0^2(0,1) \dotplus \mathrm{Span}\{\mathbf{1}, x\} \\
&= \{g \in H^2(0,1) \,|\, g'(0) = g'(1) = g(1) - g(0)\}\,.
\end{aligned}
\tag{2.5.43}
$$

(The latter boundary condition is of the form (2.5.35) with $b_1 = b_2 = -c = 1$.) S_N has not to be confused with the self-adjoint extension with Neumann boundary conditions $S_{N.bc}$, that is, the operator $S_{N.bc} = \frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with domain

$$
\mathcal{D}(S_{N.bc}) = \{g \in H^2(0,1) \,|\, g'(0) = 0 = g'(1)\}
\tag{2.5.44}
$$

and quadratic form

$$
\mathcal{D}[S_{N.bc}] = H^1(0,1)\,, \qquad S_{N.bc}[g_1, g_2] = \int_0^1 \overline{g_1'(x)}\, g_2'(x)\, \mathrm{d}x\,.
\tag{2.5.45}
$$

Although S_N and $S_{N.bc}$ have the same form domain and the same (zero) bottom, S_N is the smallest among all positive self-adjoint extensions of S (Theorem 1.3.6(i)) – the inequality $S_N[g] \leqslant S_{N.bc}[g]$ (which is strict whenever $g(0) \neq g(1)$) can be also checked explicitly by comparing (2.5.42) with (2.5.45). In fact it is easy to compute explicitly (see, e.g., [5, Example 5.1])

$$
\sigma(S_N) = \{\lambda_n \,|\, n \in \mathbb{N}\} \quad \text{with} \quad \lambda_n = \begin{cases} (n-1)^2\pi^2 & n \text{ odd} \\ k_{n/2}^2 & n \text{ even} \end{cases}
$$

$$
\sigma(S_{N.bc}) = \{(n-1)^2\pi^2 \,|\, n \in \mathbb{N}\}\,,
$$

where k_j is the unique solution to $\frac{1}{2}k = \tan(\frac{1}{2}k)$ in $(2\pi(j-1), 2\pi(j - \frac{1}{2}))$ (moreover, $k_j \to 2\pi(j - \frac{1}{2})$ as $j \to +\infty$), thus any even eigenvalue of S_N is strictly smaller then the corresponding eigenvalue of $S_{N.bc}$.

Chapter 3

Symmetries

The role of symmetries in physics is nowadays a central topic in many books. In this Chapter we stay away from very general treatments that wouldn't find here the space they deserve.

Instead we focus on a treatment of symmetries that fit questions related to the rigorous definition of quantum Hamiltonians. In the previous chapters we dealt with the problem of realising formal expressions as self-adjoint operators on Hilbert spaces. In fact, other than the formal expression of the Hamiltonian, physical reasoning often gives some considerations on the symmetry of the system.

Once a formal operator is formally invariant under a certain symmetry, there are several questions that we find naturally to ask: is this symmetry preserved when we realise the formal operator as a self-adjoint operator? In case of positive answer, how many of its self-adjoint realisations preserve the symmetry?

To answer these questions we give a rigorous definitions to these concepts in Section 3.1 and we answer them in Section 3.2.

3.1   Compact Symmetry Groups

In the context of quantum mechanics, there are many notions of symmetry, all of them having the same structure. A *symmetry* is a bijective map that preserves some mathematical structure of the space of the states of a physical system. Different notions of symmetry differ by the mathematical structure they preserve. A first notion of symmetry was proposed in 1951 by Kadison [66] in the language of C^*-algebras. Shortly speaking, Kadison requires physical symmetries to preserve the convexity of the space of states. In other words, Kadison symmetries are maps that modify the constituent states, but don't change the statistical weights of mixed states.

A second notion of symmetry is due to Wigner [121]. A Wigner symmetry is a map from the space of pure states to the space of pure states which preserves the 'transition amplitudes' (i.e. scalar products).

A third, conceptually different, type of symmetries involves time evolution. If we denote with Φ_H^t the strongly continuous one-parameter group generated by the Hamiltonian, these are maps γ that preserve one of the two above-mentioned mathematical structures and $\gamma \circ \Phi_H^t = \Phi_H^t \circ \gamma$ for any $t \in \mathbb{R}$.

Since we deal with operators that are minimally or maximally realised, usually they are not self-adjoint and then the definition of dynamical symmetry doesn't fit well with these operators.

In the case of physical systems whose states are elements of a separable Hilbert space, Wigner and Kadison symmetries are implemented as unitary or anti-unitary operators and they are the same. Hence, on this chapter, we will simply refer to symmetries as Kadison or Wigner symmetries which are also some sort of dynamical symmetries for a system whose time evolution is generated by a self-adjoint realisation of the formal operator $\widetilde{H}$.

Se we begin with the definition of symmetry

Definition 3.1.1. Consider a quantum system on the Hilbert space $\mathcal{H}$. A *symmetry* for the operator T is a unitary operator U such that

  (i) $U\mathcal{D}(T) \subset \mathcal{D}(T)$;

  (ii) $UT\psi = TU\psi$ for all $\psi \in \mathcal{D}(T)$.

In the applications, often the symmetry is mathematically implemented as a unitary representation of a group. In particular we need the following definition

Definition 3.1.2. If $(G, \star)$ is a group, a *unitary representation* of G is a map

$$\pi : G \to \mathcal{B}(\mathcal{H}) \tag{3.1.1}$$

for which

  (i) $\pi(g) = U(g)$ is a unitary operator for any $g \in G$;

  (ii) $\pi(g^{-1}) = U(g)^*$ for any $g \in G$;

  (iii) $\pi(e) = \mathbb{1}$ where e is the unit of G;

  (iv) $U(g \star h) = \pi(g \star h) = \pi(g)\pi(h) = U(g)U(h)$ for any $g, h \in G$.

In case the map π is strongly continuous in $\mathcal{H}$-topology, we say that π is a *strongly continuous unitary representation*.

We refer to Appendix A for a detailed discussion. Let us emphasize here the main results proved therein (Theorem A.2.5).

Theorem 3.1.3. *Let G be a compact Lie group and K a closed subgroup of G. Let $M = G/K$ be a homogeneous space and let $L^2(M)$ be the space of square-integrable functions over M (where M is endowed with a measure that is invariant under the action of G). The action of G is defined on $L^2(M)$ as*

$$(\lambda_g f)(x) \;:=\; f(g^{-1}x)\,. \tag{3.1.2}$$

Under these hypotheses

$$L^2(M) \;=\; \bigoplus_\alpha E_\alpha \tag{3.1.3}$$

where each E_α is a finite dimensional irreducible representation subspace of G. For $\alpha \neq \beta$, the representations $\lambda_g \restriction E_\alpha$ and $\lambda_g \restriction E_\beta$ are not equivalent.

Corollary 3.1.4. *The Hilbert space decomposition*

$$L^2(\mathbb{S}^2) \;=\; \bigoplus_{\ell \in \mathbb{N}} \mathrm{span}\,\{Y_\ell^{-\ell}, \ldots, Y_\ell^{\ell}\}\,. \tag{3.1.4}$$

Let G be a group with strongly continuous unitary representation $g \mapsto U(g)$. We say that G is a symmetry for an operator T if for all $g \in G$, $U(g)$ is a symmetry in the sense of Definition 3.1.1.

3.2 Infinite direct sum

Motivated by Theorem 3.1.3 we start the study of self-adjoint extensions of operators invariant under the action of a symmetry group by the definition of orthogonal direct sum.

Let J be a (at most) countable set and let $\mathfrak{h}_j$ be a Hilbert space for every $j \in J$. We denote with $\mathcal{H}$ the set of collections $\Psi = \{\psi_j\}_{j \in J}$ where each $\psi_j \in \mathfrak{h}_j$ and $\sum_{j \in J} \|\psi_j\|^2_{\mathfrak{h}_j} < +\infty$. Given two elements $\Phi = \{\phi_j\}_{j \in J}, \Psi = \{\psi_j\}_{j \in J} \in \mathcal{H}$ we define their scalar product in $\mathcal{H}$ as

$$\langle \Psi, \Phi \rangle_{\mathcal{H}} = \sum_{j \in J} \langle \psi_j, \phi_j \rangle_{\mathfrak{h}_j}. \tag{3.2.1}$$

It is a standard fact that, with these definitions, $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is a Hilbert space. With respect to this decomposition, we will call each $\mathfrak{h}_j$ a fibre and each ψ_j the j-th component of Ψ. It follows immediately from definitions that two elements $\Psi, \Phi \in \mathcal{H}$ supported on disjoint fibres are orthogonal. This fact justifies the introduction of the notation

$$\Psi = \oplus_{j \in J} \psi_j \tag{3.2.2}$$

instead of $\Psi = \{\psi_j\}_{j \in J}$.

It is also customary to use the notation

$$\mathcal{H} = \bigoplus_{j \in J} \mathfrak{h}_j \tag{3.2.3}$$

for the Hilbert space.

If $T : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}$ is an operator and $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, we say that $\mathcal{H}_1$ is a reducing subspace for T if $T(\mathcal{D}(T) \cap \mathcal{H}_1) \subset \mathcal{H}_1$ and $T(\mathcal{D}(T) \cap \mathcal{H}_1 \perp) \subset \mathcal{H}_1^\perp$.

Definition 3.2.1. A not necessarily unbounded operator $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$ is said to be *maximally decomposable* if

i) Each $\mathfrak{h}_j$ is a reducing subspace for A and we call $A_j := A \upharpoonright_{\mathfrak{h}_j}$

ii)
$$\mathcal{D}(A) = \left\{ \Psi \in \mathcal{H} \middle| \begin{array}{c} \psi_j \in \mathcal{D}(A_j) \\ \sum_{j \in J} \|A_j \psi_j\|^2_{\mathfrak{h}_j} < +\infty \end{array} \right\}$$

with $\mathcal{D}(A_j) = \mathcal{D}(A) \cap \mathfrak{h}_j$.

Lemma 3.2.2. *If A is a bounded operator defined on $\mathcal{H}$ that is reduced by any $\mathfrak{h}_j$, then A is maximally decomposable.*

Proof. Condition ii) of Definition 3.2.1 follows by boundedness. Indeed

$$\sum_{j \in J} \|A_j \psi_j\|^2_{\mathfrak{h}_j} = \|A\Psi\|^2_{\mathcal{H}} \leqslant C \|\Psi\|^2_{\mathcal{H}} < +\infty$$

$\square$

Remark 3.2.3. Lemma 3.2.2 says that the distinction among maximally decomposable and reducible operators is proper for unbounded operators. It is not true that any reducible unbounded operator is also maximally decomposable (see Definition 3.2.23 later).

As a trivial example let us consider on $\ell^2(\mathbb{Z}) = \bigoplus_{j \in \mathbb{Z}} \mathbb{C}$ the following operators:

$$\begin{array}{ll} A : (A\Psi) = \oplus_{j \in \mathbb{Z}} j\psi_j & \mathcal{D}(A) = \{\Psi \in \ell^2(\mathbb{Z}) \mid \sum_{j \in J} |j|^2 |\psi_j|^2 < +\infty\} \\ B : (B\Psi) = \oplus_{j \in \mathbb{Z}} j\psi_j & \mathcal{D}(B) = \{\Psi \in \ell^2(\mathbb{Z}) \mid \sum_{j \in J} |j|^{2a} |\psi_j|^2 < +\infty \, \forall a \in \mathbb{N}\} \\ C : (C\Psi) = \oplus_{j \in \mathbb{Z}} j\psi_j & \mathcal{D}(C) = \{\Psi \in \ell^2(\mathbb{Z}) \mid \psi_j \neq 0 \, \text{for finitely many j}\}. \end{array} \tag{3.2.4}$$

All these operators are reduced, but only A is decomposed.

Lemma 3.2.4. *Let A be a maximally decomposable operator, then A is densely defined in $\mathcal{H}$ if and only if each A_j is densely defined in $\mathfrak{h}_j$.*

Proof. The thesis is a consequence of the following chain of equalities which holds trivially when the closure is taken in the $\| \cdot \|_{\mathcal{H}}$- norm:

$$\overline{\mathcal{D}(A)} = \overline{\bigoplus_{j \in J} \mathcal{D}(A_j)} = \bigoplus_{j \in J} \overline{\mathcal{D}(A_j)}.$$

□

Lemma 3.2.5. *If A is a bounded and maximally decomposable operator then each A_j is bounded with $\|A_j\|_{op} \leqslant \|A\|_{op}$.*

Proof. Since each $A_j = A \upharpoonright_{\mathfrak{h}_j}$ the thesis follows.   □

Remark 3.2.6. The converse of Lemma is not true. Indeed there exists operator whose fibres are bounded but the overall operator is not. As an example, take any of the operators in (3.2.4). Under the additional hypothesis that A_j are uniformly bounded in j, the converse is true.

Lemma 3.2.7. *Let A be a maximally decomposable operator. A is bounded if and only if each A_j is uniformly bounded with respect to $j \in J$.*

Proof. One implication is proved as Lemma 3.2.6. For the opposite, if each A_j is uniformly bounded it means that $\|A_j\|_{op} < C$ with C independent of j. Then

$$\|A\Psi\|_{\mathcal{H}} = \sum_{j \in J} \|A_j \psi_j\|_{\mathfrak{h}_j}^2 \leqslant C \sum_{j \in J} \|\psi_j\|_{\mathfrak{h}_j}^2 = C\|\Psi\|_{\mathcal{H}}^2.$$

□

Proposition 3.2.8. *Let A be a densely defined maximally decomposable operator, then*

  i) A^*, its adjoint, is well defined;

  ii) A^* is maximally decomposable and, in particular,

$$\mathcal{D}(A^*) = \left\{ \Psi \in \mathcal{H} \,\middle|\, \begin{array}{c} \psi_j \in \mathcal{D}((A_j)^*) \\ \sum_{j \in J} \|A_j^* \psi_j\|_{\mathfrak{h}_j}^2 < +\infty \end{array} \right\} \tag{3.2.5}$$

Proof. To prove that A^* is maximally decomposable we show first that $\mathfrak{h}_j$ is a reducing subspace for A^* and for any $j \in J$. To this aim let us pick up $\Psi \in \mathcal{D}(A^*) \cap \mathfrak{h}_j$. For any $\Phi \in \mathcal{D}(A)$

$$\langle A^*\Psi, \Phi \rangle_{\mathcal{H}} = \langle \Psi, A\Phi \rangle_{\mathcal{H}} = \langle \Psi, A_j\phi_j \rangle_{\mathfrak{h}_j}.$$

From this equality we see that if $\Phi \in \mathfrak{h}_j^\perp$ then $\phi_j = 0$ and $\langle A^*\Psi, \Phi \rangle_{\mathcal{H}} = 0$. Since A is densely defined, this implies that $A^*\Psi \in \mathfrak{h}_j$.

It remains to prove that if $\Psi \in \mathcal{D}(A^*) \cap (\mathfrak{h}_j^\perp)$ then $A^*\Psi \in \mathfrak{h}_j^\perp$. Let us pick up $\Phi \in \mathcal{D}(A) \cap \mathfrak{h}_j$. Then

$$\langle A^*\Psi, \Phi \rangle_{\mathcal{H}} = \langle \Psi, A\Phi \rangle_{\mathcal{H}} = 0$$

the last term vanishes because A is maximally decomposable and hence $A\Phi \in \mathfrak{h}_j$, while $\Psi \in \mathfrak{h}_j^\perp$. At this point we proved that $\mathfrak{h}_j$ is a reducing subspace for A for any $j \in J$.

We now define

$$\mathcal{D} := \left\{ \Psi \in \mathcal{H} \,\middle|\, \begin{array}{c} \psi_j \in \mathcal{D}((A_j)^*) \\ \sum_{j \in J} \|A_j^* \psi_j\|_{\mathfrak{h}_j}^2 < +\infty \end{array} \right\}.$$

To prove decomposability it is sufficient to show that $\mathcal{D} = \mathcal{D}(A^*)$. We start with the inclusion $\mathcal{D}(A^*) \supset \mathcal{D}$. Take $\Psi \in \mathcal{D}$, we want to show that $\forall \Phi \in \mathcal{D}(A)$ there exists $\chi \in \mathcal{H}$ such that $\langle \chi, \Phi \rangle_{\mathcal{H}} = \langle \Psi, A\Phi \rangle_{\mathcal{H}}$. Indeed

$$\langle \Psi, A\Phi \rangle_{\mathcal{H}} = \sum_{j \in J} \langle \psi_j, A_j \phi_j \rangle_{\mathfrak{h}_j} = \sum_{j \in J} \langle (A_j)^* \psi_j, \phi_j \rangle_{\mathfrak{h}_j} = \langle \oplus_{j \in J} ((A_j)^* \psi_j), \Phi \rangle_{\mathcal{H}}$$

in the second equality we used $\psi_j \in \mathcal{D}((A_j)^*)$ and $\oplus_{j \in J} (A_j)^* \psi_j \in \mathcal{H}$ because of the second condition in $\mathcal{D}$.

For the converse inclusion, let us pick up $\Psi \in \mathcal{D}(A^*)$. Since A^* is reduced by $\mathfrak{h}_j$, this means that each $\psi_j \in \mathcal{D}(A^*)$. So, for any $\Phi \in \mathcal{D}(A)$,

$$\langle A^* \psi_j, \Phi \rangle_{\mathcal{H}} = \langle \psi_j, A\Phi \rangle_{\mathcal{H}} = \langle \psi_j, A_j \phi_j \rangle_{\mathfrak{h}_j} .$$

Since $A^* \psi_j \in \mathfrak{h}_j$ the chain of equalities proves that if $\Psi \in \mathcal{D}(A^*)$, then $\psi_j \in \mathcal{D}((A_j)^*)$ and $A^* \psi_j = A_j^* \psi_j$.

Last,

$$+\infty > \|A^* \Psi\|_{\mathcal{H}}^2 = \sum_{j \in J} \|A_j^* \psi_j\|_{\mathfrak{h}_j}^2 .$$

$\square$

Remark 3.2.9. As a consequence of this proposition, we can say that if A is maximally decomposable and densely defined, $(A_j)^* = (A^*)_j$. In particular this will make unambiguous the notation A_j^*.

Lemma 3.2.10. *Let A be a densely defined maximally decomposable operator, then A is closable if and only if each A_j is closable and A is closed if and only if each A_j is closed.*

Proof. If A is closable, from [104, Theorem 1.8 (i)], we know that $\mathcal{D}(A^*)$ is dense and hence, by (3.2.5), each $\mathcal{D}(A_j^*)$ is dense in $\mathfrak{h}_j$ implying that each A_j is closable. For the opposite, suppose that each A_j is closable, then $\mathcal{D}(A_j^*)$ is dense in $\mathfrak{h}_j$ and by (3.2.5) also $\mathcal{D}(A^*)$ is dense in $\mathcal{H}$ whence the closability of A follows from [104, Theorem 1.8 (i)].

If A is closed then $A = A^{**}$ and from (3.2.5) we deduce that $A_j = A_j^{**}$ for any j whence the closure of each A_j. Conversely, if each A_j is closed then $A_j^{**} = A_j$ and hence $A^{**} = A$ proving the closedness of A. $\square$

Lemma 3.2.11. *Let A be a closed maximally decomposable operator on $\mathcal{H}$. Then, if $\lambda \in \mathbb{C}$,*

$$\ker(A - \lambda \mathbb{1}_{\mathcal{H}}) = \bigoplus_{j \in J} \ker(A_j - \lambda \mathbb{1}_j) \tag{3.2.6}$$

Proof. The inclusion $\bigoplus_{j \in J} \ker(A_j - \lambda \mathbb{1}) \subset \ker(A - \lambda \mathbb{1})$ is trivial. For the opposite, let us pick up $\Psi \in \ker(A - \lambda \mathbb{1})$. Then

$$0 = \|(A - \lambda \mathbb{1})\Psi\|_{\mathcal{H}}^2 = \sum_{j \in J} \|(A_j - \lambda \mathbb{1}_j)\psi_j\|_{\mathfrak{h}_j}^2 .$$

Since the latter is the sum of positive terms, its vanishing implies the vanishing of each of the summands identically. This implies that $\psi_j \in \ker(A_j - \lambda \mathbb{1}_j)$ for each $j \in J$. $\square$

Lemma 3.2.12. *Let A be a densely defined maximally decomposable operator. Then A is symmetric if and only if A_j is symmetric for every $j \in J$.*

Proof. By definition, if A is symmetric, for every $\Psi, \Phi \in \mathcal{D}(A)$ we have $\langle \Psi, A\Phi \rangle_{\mathcal{H}} = \langle A\Psi, \Phi \rangle_{\mathcal{H}}$. This in particular holds when $\Psi, \Phi \in \mathcal{D}(A_j)$ proving symmetry of A_j.

For the contrary let us argue by contradiction. Let us suppose that for some $j_0 \in J$, A_{j_0} is not symmetric. This implies that there exists $\Psi, \Phi \in \mathcal{D}(A_{j_0})$ s.t. $\langle \Psi, A_{j_0}\phi \rangle_{\mathcal{H}} \neq \langle \Psi, A_{j_0}\Phi \rangle_{\mathcal{H}}$. Since $\Psi, \Phi \in \mathcal{D}(A)$ and hence we found a pair of functions in the domain of A for which A is not symmetric. Therefore A is not symmetric, completing the proof. $\square$

From now on we consider two scalar products on $\mathcal{D}(A)$, i.e. the enviromental Hilbert space scalar product defined by (3.2.1) and the graph scalar product of A

$$\langle \Psi, \Phi \rangle_A := \langle A\Psi, A\Phi \rangle_{\mathcal{H}} + \langle \Psi, \Phi \rangle_{\mathcal{H}}, \qquad \Psi, \Phi \in \mathcal{D}(A). \tag{3.2.7}$$

To keep consistency with the other parts of the text, the symbols $\oplus, \boxplus$ without any label denotes orthogonality with respect to the enviromental Hilbert scalar product, while $\oplus^A, \boxplus^A$ will denote orthogonality with respect to the graph scalar product of A. We will keep the notation $\dot{+}$ for the direct sum of vector spaces that are not known a priori to be orthogonal one to each other.

Lemma 3.2.13. *Let A be a densely defined symmetric maximally decomposable operator on $\mathcal{H}$; then*

$$\mathcal{D}(A^*) = \Big(\bigoplus_{j \in J}^{A^*} \mathcal{D}(\overline{A_j}) \Big) \oplus^{A^*} \ker(A^* - \mathrm{i}\mathbb{1}) \oplus^{A^*} \ker(A^* + \mathrm{i}\mathbb{1}) \tag{3.2.8}$$

Proof. Due to Proposition 3.2.8, A^* is a closed maximally decomposable operator. Therefore

$$\mathcal{D}(A^*) = \bigoplus_{j \in J}^{A^*} \mathcal{D}(A_j^*)$$

Using von Neumann's decomposition [95, Lemma p.138] for $\mathcal{D}(A_j^*)$, we obtain

$$\mathcal{D}(A^*) = \bigoplus_{j \in J}^{A^*} \Big(\mathcal{D}(\overline{A_j}) \oplus^{A^*} \ker(A_j^* + \mathrm{i}\mathbb{1}_j) \oplus^{A^*} \ker(A_j^* - \mathrm{i}\mathbb{1}_j) \Big) .$$

Using distributivity of the direct sum $\oplus^{A^*}$ and Lemma 3.2.11 we obtain the thesis. $\square$

Lemma 3.2.14. *Let A be a densely defined symmetric maximally decomposable operator on $\mathcal{H}$. Then*

$$\mathcal{D}(\overline{A}) = \boxplus_{j \in J} \mathcal{D}(\overline{A_j}) \tag{3.2.9}$$

Proof. It follows from Proposition 3.2.8 by taking the double adjoint of A. $\square$

Lemma 3.2.15. *Let A be a densely defined symmetric decomposable operator on $\mathcal{H}$. Then*

$$\mathcal{D}(A^*) = (\boxplus_{j \in J} \mathcal{D}(\overline{A_j})) \dot{+} \ker(A^* - \mathrm{i}\mathbb{1}) \dot{+} \ker(A^* + \mathrm{i}\mathbb{1}) \tag{3.2.10}$$

Proof. We obtain the thesis directly from Lemmas 3.2.13 and 3.2.14. $\square$

Lemma 3.2.16. *Let A be a densely defined maximally decomposable operator on $\mathcal{H}$. Then if A is invertible on $\mathcal{H}$, each A_j is invertible on $\mathfrak{h}_j$ and A^{-1} is maximally decomposable.*

Proof. Suppose A is invertible on $\mathcal{H}$, i.e. for any $\Psi \in \mathcal{H}$ there exists a unique $\Phi \in \mathcal{H}$ s.t. $A\Phi = \Psi$. In particular, if $\Psi \in \mathfrak{h}_j$ then $\Phi \in \mathcal{D}(A_j)$. Indeed let us suppose that $\Phi_\ell \neq 0$ for some $\ell \neq j$. $A\Phi_\ell = A_\ell \Phi_\ell = \Psi_\ell = 0$, therefore $\Phi_\ell = 0$ since $\ker A = \{0\}$. Hence $\Phi \in \mathcal{D}(A_j)$. At this point we proved that $A^{-1} \restriction_{\mathfrak{h}_j}$ inverts A_j and hence A_j is invertible.

We have to prove that A^{-1} is maximally decomposable. The previous argument showed also that A^{-1} is reduced by the Hilbert space decomposition $\bigoplus_{j \in J} \mathfrak{h}_j$. Since A^{-1} is bounded, this is sufficient for A^{-1} to be maximally decomposable.

$\square$

Remark 3.2.17. The converse of Lemma 3.2.16 is not true. Namely we can construct a maximally decomposable operator which is not invertible on the whole $\mathcal{H}$ and whose fibers A_j are all invertible. Let us consider

$$\mathcal{H} = \ell^2(\mathbb{N}) = \bigoplus_{j=1}^{+\infty} \mathbb{C} \tag{3.2.11}$$

We consider the bounded operator $A : \ell^2(\mathbb{N}) \to \ell^2(\mathbb{N})$ which acts as follows

$$y_j = (Ax)_j = A_j x_j = \frac{1}{j} x_j. \tag{3.2.12}$$

It is clear that each A_j is invertible, i.e.

$$x_j = (A^{-1}y)_j = A_j^{-1} y_j = j y_j. \tag{3.2.13}$$

But the operator $A = \bigoplus_{j \in J} A_j$ is not invertible on $\mathcal{H}$ because $\sigma(A) = \{\frac{1}{j} \mid j = 1, 2, \dots\} \cup \{0\}$.

Lemma 3.2.18. *Let A be a closed densely defined maximally decomposable operator on $\mathcal{H}$. If $\lambda \in \rho(A)$ then $\lambda \in \rho(A_j)$ for all $j \in J$.*

Proof. The fact that $\lambda \in \rho(A)$ means that $(A - \lambda)$ is invertible on $\mathcal{H}$. Due to Lemma 3.2.16 $(A_j - \lambda \mathbb{1}_j)$ is also invertible and hence $\lambda \in \rho(A_j)$ for any $j \in J$. $\square$

Remark 3.2.19. With an argument similar to the one exposed in the previous Remark, one can prove that there can be $\lambda \in \rho(A_j)$ for any j with $\lambda \notin \rho(A)$.

Lemma 3.2.20. *Let A be a densely defined symmetric maximally decomposable operator on $\mathcal{H}$. Then it admits maximally decomposable self-adjoint extensions if and only if $\ker(A_j^* - \mathrm{i}\mathbb{1}_j) \cong \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$ for any $j \in J$.*

Proof. Suppose that A_U is a self-adjoint extension of A which is maximally decomposable according to $\mathcal{H} = \bigoplus_{j \in J} \mathfrak{h}_j$. Since A_U is maximally decomposable, each $\mathfrak{h}_j$ is a reducing subspace for A_U and for every $j \in J$ we can define the operators $A_{U,j} := A_U \upharpoonright \mathfrak{h}_j$ with $\mathcal{D}(A_{U,j}) = \mathcal{D}(A_U) \cap \mathfrak{h}_j$. Moreover $\mathcal{D}(A_{U,j}) \subset \mathcal{D}(A_U)$. We can pick up a generic $\Psi \in \mathcal{D}(A_{U,j})$. For such a $\Psi = \oplus_{j \in J} \psi_j$, we have $\psi_\ell = 0$ for all $\ell \neq 0$. If $\psi_\ell = 0$ this implies that all the components of ψ_ℓ (the one on $\mathcal{D}(\overline{A_\ell})$ and $\ker(A^* \pm \mathrm{i}\mathbb{1}_j)$) vanishes because of linear independence of vectors in these three linear spaces. This proves that since $\psi_j = \varphi + \varphi_+ + U\varphi_+$ is the only non-zero component, that $U : \ker(A_j^* - \mathrm{i}\mathbb{1}_j) \to \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$.

Repeating the same argument one can prove that all $\ker(A_j^* - \mathrm{i}\mathbb{1}_j)$ are reducing subspaces for U and, since U is unitary, it is in particular bounded and Lemma 3.2.2 implies that it is maximally decomposable. We have thus constructed a family of unitary operators U_j, which maps, for any j $\ker(A_j^* - \mathrm{i}\mathbb{1}_j) \to \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$. Therefore $\ker(A_j^* - \mathrm{i}\mathbb{1}_j) \cong \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$ for any $j \in J$.

For the opposite, if $\ker(A_j^* - \mathrm{i}\mathbb{1}_j) \cong \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$, then we can construct, for any $j \in J$, a unitary operator $U_j : \ker(A_j^* - \mathrm{i}\mathbb{1}_j) \to \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$ and a unitary operator $U := \oplus_{j \in J} U_j$. We want to prove that A_U is a maximally decomposable self-adjoint extension of U. It is self-adjoint because of von Neumann's theorem [95, Theorem X.2]. To show that it is maximally decomposable we have to show that $\mathcal{D}(A_{U,j}) := \mathcal{D}(A_U) \cap \mathfrak{h}_j \subset \mathcal{D}(A_{U,j})$.

Let us pick up $\Psi \in \mathcal{D}(A_{U,j})$. Then we can decompose $\Psi = \oplus_{\ell \in J}(\varphi_\ell + \varphi_{+,\ell} + U\varphi_{+,\ell})$. For $\ell \neq 0$, $\psi_\ell = 0$ and hence both φ_ℓ and $\varphi_{+,\ell}$ vanishes because they are linearly independent vectors. Hence, if $\Psi = \Phi + \Phi_+ + U\Phi_+$ and $\Psi \in \mathcal{D}(A_{U,j})$ then $\Phi \in \mathcal{D}(\overline{A_j})$, $\Phi_+ \in \ker(A_j^* - \mathrm{i}\mathbb{1}_j)$ and $U\Phi_+ \in \ker(A_j^* + \mathrm{i}\mathbb{1}_j)$. Now we check that $A_U \Psi \in \mathfrak{h}_j$. Indeed

$$A_U \Psi = \overline{A}\Phi + \mathrm{i}\Phi_+ - \mathrm{i}U\Phi_+ = \overline{A_j}\Phi + \mathrm{i}\Phi_+ - \mathrm{i}U_j\Phi_+$$

where the latter is the sum of three vectors in $\mathfrak{h}_j$. Therefore $A_U \Psi \in \mathfrak{h}_j$.

With the same argument one proves that $\mathfrak{h}_j^\perp$ is a reducing subspace for A_U, completing the proof of decomposability of A_U. $\square$

Remark 3.2.21. It may happen that a maximally decomposable operator has only self-adjoint extensions which are not maximally decomposable. Indeed let us pick up $A = -i\frac{d}{dx}$ on $H_0^1(\mathbb{R} \setminus \{0\}) \subset L^2(\mathbb{R})$. In this case, the operator is maximally decomposable according to $L^2(\mathbb{R}) \cong L^2((-\infty, 0), dx) \oplus L^2((0, +\infty), dx)$, $A \cong A_1 \oplus A_2$. With a straightforward computation one can see that

$$
\begin{aligned}
\ker(A_1^* + i\mathbb{1}) &= \mathrm{span}_{\mathbb{C}}\{e^x\}, & \ker(A_1^* - i\mathbb{1}) &= \{0\} \\
\ker(A_2^* + i\mathbb{1}) &= \{0\} & \ker(A_2^* - i\mathbb{1}) &= \mathrm{span}_{\mathbb{C}}\{e^{-x}\}.
\end{aligned}
\tag{3.2.14}
$$

Thus all self-adjoint extensions are obtained with unitary operators that are not reduced by the original Hilbert space decomposition.

Corollary 3.2.22. *Let A be a densely defined, symmetric and maximally decomposable operator on $\mathcal{H}$ which admits self-adjoint extensions. All its self-adjoint extensions are maximally decomposable if and only if for at most one $j_0 \in J$, $\ker(A_{j_0}^* - i\mathbb{1}_{j_0}) \neq \{0\}$ and $\ker(A_{j_0}^* + i\mathbb{1}_{j_0}) \neq \{0\}$.*

Proof. If $\ker(A_j^* \pm i\mathbb{1}_j) = \{0\}$ for all $j \in J$, then A is essentially self-adjoint and it admits only one self-adjoint extension: its closure. Its closure is maximally decomposable because of Lemma 3.2.14.

If $\ker(A_{j_0}^* + i\mathbb{1}_{j_0}) \neq \{0\}$ and $\ker(A_{j_0}^* - i\mathbb{1}_{j_0}) \neq \{0\}$ for just one $j_0 \in J$, then any unitary $U : \ker(A^* + i\mathbb{1}) \to \ker(A^* - i\mathbb{1})$ maps a (Hilbert) subspace of $\mathfrak{h}_{j_0}$ into another (Hilbert) subspace of $\mathfrak{h}_{j_0}$. Such a unitaries exist because the two deficiency spaces are isomorphic (otherwise A would not admit self-adjoint extensions).

In this case, it is obvious that for any self-adjoint extension of A, $\mathfrak{h}_{j_0}$ is a reducing subspace. It is obvious aswell that each $\mathfrak{h}_j$ is a reducing subspace because the self-adjoint extension of the operator $A \upharpoonright_{\mathfrak{h}_{j_0}^\perp}$ is its closure.

To prove the contrary we argue by contradiction. Let us suppose there exists a self-adjoint extension which is maximally decomposable. If it does not exists the thesis is trivial. Let us call A_U the maximally decomposable self-adjoint extension. Here $U : \ker(A^* - i\mathbb{1}) \to \ker(A^* + i\mathbb{1})$. Using now Lemma 3.2.20 and the hypothesis, we know that there exists a pair of indices $j_1, j_2 \in J$ for which the defect spaces of A_{j_1} and A_{j_2} are not trivial and isomporphic. Let us pick up a one dimensional subspace $V_{j_1} \subset \ker(A_{j_1}^* + i\mathbb{1}_{j_1})$ and a one-dimensional subspace $V_{j_2} \subset \ker(A_{j_2}^* + i\mathbb{1}_{j_2})$. We call a unitary $W : V_{j_1} \to V_{j_2}$. Then $W \oplus W^*$ is a unitary operator from $V_{j_1} \oplus V_{j_2}$ into itself. The self-adjoint extension A_{WU} is not maximally decomposable because $\mathfrak{h}_{j_1}$ and $\mathfrak{h}_{j_2}$ are not reducing subspaces. $\square$

Often, in concrete problems, one don't start by extending an operator whose domain is of the form of Definition 3.2.1, so it is useful to introduce a second operator, smaller than the maximally decomposable one, with the property that they have the same closure.

Definition 3.2.23. A not necessarily unbounded operator $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$ is said to be *minimally decomposable* if

  i) Each $\mathfrak{h}_j$ is a reducing subspace for A and we call $A_j := A \upharpoonright_{\mathfrak{h}_j}$

 ii)
$$
\mathcal{D}(A) = \left\{ \Psi \in \mathcal{H} \middle| \begin{array}{c} \psi_j \in \mathcal{D}(A_j) \\ \psi_j \neq 0 \text{ for finitely many } j \in J \end{array} \right\}
$$

   with $\mathcal{D}(A_j) = \mathcal{D}(A) \cap \mathfrak{h}_j$.

Remark 3.2.24. If A_1 and A_2 are two densely defined operator and A_1 is maximally decomposable, A_2 is minimally decomposable and $A_1 = A_2$ on $\mathcal{D}(A_2)$ then clearly $A_2 \subset A_1$.

Lemma 3.2.25. *If A_1 and A_2 are two densely defined operators on $\mathcal{H} = \bigoplus_{j \in J} \mathfrak{h}_j$, A_1 is maximally decomposable, A_2 is minimally decomposable and $A_1 = A_2$ on $\mathcal{D}(A_2)$, then $\overline{A_1} = \overline{A_2}$.*

Proof. We prove this fact by showing that $A_1^* = A_2^*$. This implies the thesis because $A_1^{**} = \overline{A_1}$ (see [104, Theorem 1.8]).

Since $A_2 \subset A_1$ then it is only necessary to prove that $A_2^* \subset A_1^*$.

We start by showing that A_2^* is reduced by any $\mathfrak{h}_j$. Let us pick up $\Psi \in \mathcal{D}(A_2^*) \cap \mathfrak{h}_j$ and $\Phi \in \mathcal{D}(A_2) \cap (\mathfrak{h}_j^\perp)$. Then

$$\langle A_2^* \Psi, \Phi \rangle_{\mathcal{H}} = \langle \Psi, A_2 \Phi \rangle_{\mathcal{H}} = \sum_{j \in J} \langle \psi_j, A_{2,j} \phi_j \rangle_{\mathfrak{h}_j} = 0$$

This computation shows that $\mathfrak{h}_j$ is an invariant subspace for A_2^*. With the same argument one can conclude that also $\mathfrak{h}_j^\perp$ is an invariant subspace for A_2^* and since this argument holds for any $j \in J$ one concludes that each $\mathfrak{h}_j$ is an invariant subspace for A_2^*.

To prove that $A_2^* \subset A_1^*$ now it is sufficient to prove that if $\Psi \in \mathcal{D}(A_2^*)$ then $\psi_j \in \mathcal{D}(A_{1,j}^*)$ and $A_{2,j}^* \psi_j = A_{1,j}^* \psi_j$ for any $j \in J$.

Let us take $\Psi \in \mathcal{D}(A_2^*)$ and $\Phi \in \mathcal{D}(A_2) \restriction_{\mathfrak{h}_j} = \mathcal{D}(A_1) \restriction_{\mathfrak{h}_j}$. Then

$$\langle A_2^* \Psi, \Phi \rangle_{\mathcal{H}} = \langle \psi_j, A_{2,j} \phi_j \rangle_{\mathfrak{h}_j} = \langle \psi_j, A_{1,j} \phi_j \rangle_{\mathfrak{h}_j} = \langle A_{1,j}^* \psi_j, \phi_j \rangle_{\mathfrak{h}_j}$$

This proves that $\psi_j \in \mathcal{D}(A_{1,j}^*)$ for any $j \in J$ and that $A_{2,j}^* = A_{1,j}^*$ for any $j \in J$. Therefore

$$+\infty > \|A_2^* \Psi\|_{\mathcal{H}}^2 = \sum_{j \in J} \|A_{2,j}^* \psi_j\|_{\mathfrak{h}_j}^2 = \sum_{j \in J} \|A_{1,j}^* \psi_j\|_{\mathfrak{h}_j}^2.$$

$\square$

Remark 3.2.26. Lemma 3.2.25 is very important for concrete applications because often we have to study self-adjoint realisations of operators that are in the between a maximally decomposable one and a minimally decomposable one. If this is the case, the self-adjoint extension of the concrete operator we are dealing with are the same of its maximally decomposable extension.

Lemma 3.2.27. *Let A be a self-adjoint and maximally decomposable operator on $\mathcal{H}$. The following equality holds*

$$\rho(A) = \mathrm{int}\left(\bigcap_{j \in J} \rho(A_j)\right) \tag{3.2.15}$$

where int *denotes the interior of the set.*

Proof. The fact that $\rho(A) \subset \rho(A_j)$ for any $j \in J$ follows from Lemma 3.2.18 and then, it trivially follows that $\rho(A) \subset \cap_{j \in J} \rho(A_j)$. Since $\rho(A) = \mathrm{int}\,\rho(A)$, since the resolvent set is open, then $\rho(A) \subset \mathrm{int}\left(\bigcap_{j \in J} \rho(A_j)\right)$.

Now, to see that $\mathrm{int} \cap_{j \in J} \rho(A_j) \subset \rho(A)$ we show that $(A - \lambda \mathbb{1})^{-1}$ exists and it is bounded if $\lambda \in \mathrm{int} \cap_{j \in J} \rho(A_j)$.

Indeed, if $\lambda \in \cap_{j \in J} \rho(A_j)$ we know that $A_j - \lambda \mathbb{1}_j$ is invertible on the whole $\mathfrak{h}_j$. Since now $\lambda \in \mathrm{int}(\cap_{j \in J} \rho(A_j))$ then there exists $\varepsilon > 0$ s.t. $\mathrm{dist}\,(\lambda, \mathbb{C} \setminus \cap_{j \in J} \rho(A_j)) > \varepsilon$.

Let us call $\mathcal{D} := \{\Psi \in \mathcal{H} \,|\, \psi_j \neq 0$ for finitely many $j\}$. $\mathcal{D}$ is dense in $\mathcal{H}$. The operator $\bigoplus_{j \in J} (A_j - \lambda \mathbb{1}_j)^{-1}$ is well defined on $\mathcal{D}$. Moreover it is bounded, i.e.

$$\|\bigoplus_{j \in J} (A_j - \lambda \mathbb{1}_j)^{-1}\|_{op} \leqslant \frac{1}{\varepsilon}$$

because of a standard resolvent estimate. Therefore it extends uniquely to a bounded operator $(A - \lambda \mathbb{1})^{-1} : \mathcal{H} \to \mathcal{D}(A)$. This completes the proof that $\lambda \in \rho(A)$. $\square$

Corollary 3.2.28. *Let A be a closed and maximally decomposable operator on $\mathcal{H}$. Then*

$$\sigma(A) = \overline{\bigcup_{j \in J} \sigma(A_j)} \tag{3.2.16}$$

Proof. The proof follows from Lemma 3.2.27. $\qquad\square$

Part II

Applications to Quantum Mechanical models

Chapter 4

Hydrogen Hamiltonians with point-like perturbation at the centre

4.1 Outlook and Main Results

As a first example of quantum mechanical Hamiltonian with symmetry, we are concerned with certain realistic types of perturbations of the familiar quantum Hamiltonian for the valence electron of hydrogenoid atoms, namely the operator

$$H_{\text{Hydr}} \;=\; -\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{|x|} \tag{4.1.1}$$

on $L^2(\mathbb{R}^3)$ with domain of self-adjointness $H^2(\mathbb{R}^3)$, where m and $-e$ are, respectively, the electron's mass and charge ($e > 0$), Z is the atomic number of the nucleus, $\hbar$ is Planck's constant and Δ is the three-dimensional Laplacian.

In particular, we are concerned with the deviations from the celebrated spectrum of the hydrogen atom:

$$\sigma_{\text{ess}}(H_{\text{Hydr}}) \;=\; \sigma_{\text{ac}}(H_{\text{Hydr}}) \;=\; [0, +\infty)\,, \quad \sigma_{\text{sc}}(H_{\text{Hydr}}) \;=\; \varnothing$$
$$\sigma_{\text{point}}(H_{\text{Hydr}}) \;=\; \Big\{ -mc^2 \frac{(Z\alpha_{\text{f}})^2}{2n^2} \,\Big|\, n \in \mathbb{N} \Big\} \tag{4.1.2}$$

where $\alpha_{\text{f}} = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the fine structure constant and c is the speed of light.

Intimately related to this problem, we are concerned with the problem of the self-adjoint realisations of the 'radial' differential operator

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\nu}{r}\,, \qquad \nu \in \mathbb{R} \tag{4.1.3}$$

on the Hilbert space of the half-line, $L^2(\mathbb{R}^+, \mathrm{d}r)$, and on the classification of all such realisations and the characterisation of their spectra.

4.1.1 Point-like perturbations supported at the interaction centre

As well known [12, §34], standard calculations within first-order perturbation theory, made first by Sommerfeld even before the complete definition of quantum mechanics, show that the correction

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$\delta E_n^{(\mathrm{H})}$ to the n-th eigenvalue $E_n^{(\mathrm{H})} := -\frac{(Z\alpha_{\mathrm{f}})^2}{2n^2}$ of (4.1.2) is given by

$$\frac{\delta E_n^{(\mathrm{H})}}{E_n^{(\mathrm{H})}} \;=\; -\frac{(Z\alpha_{\mathrm{f}})^2}{n}\Big(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\Big), \tag{4.1.4}$$

where j is the quantum number of the total angular momentum, thus $j = \frac{1}{2}$ if $\ell = 0$ and $j = \ell \pm \frac{1}{2}$ otherwise, in the standard notation that we shall remind in a moment. (The net effect is therefore a partial removal of the degeneracy of $E_n^{(\mathrm{H})}$ in the spin of the electron and in the angular number ℓ, a double degeneracy remaining for levels with the same n and $\ell = j \pm \frac{1}{2}$, apart from the maximum possible value $j_{\max} = n - \frac{1}{2}$.)

Let us recall (see, e.g., [111, Chapter 6]) that the first-order perturbative scheme yielding (4.1.4) corresponds to adding to H_{Hydr} corrections that arise in the non-relativistic limit from the Dirac operator for the considered atom: H_{Hydr} is indeed formally recovered as one of the two identical copies of the spinor Hamiltonian obtained from the Dirac operator as $c \to +\infty$, and the eigenvalues of the latter, once the rest energy mc^2 is removed, converge to those of H_{Hydr}, with three types of subleading corrections, to the first order in $1/c^2$:

- the *kinetic energy correction*, interpreted in terms of the replacement of the relativistic with the non-relativistic energy, that classically amounts to the contribution

$$\Big(\sqrt{c^2 p^2 - m^2 c^4} - mc^2\Big) - \frac{p^2}{2m} \;=\; -\frac{1}{8m^2 c^2} p^4 + O(c^{-4})\,;$$

- the *spin-orbit correction*, interpreted in terms of the interaction of the magnetic moment of the electron with the magnetic field generated by the nucleus in the reference frame of the former, including also the effect of the Thomas precession;

- the *Darwin term correction*, interpreted as an effective smearing out of the electrostatic interaction between the electron and nucleus due to the Zitterbewegung, the rapid quantum oscillations of the electron.

In fact, each such modified eigenvalue $E_n^{(\mathrm{H})} + \delta E_n^{(\mathrm{H})}$ is the first-order term of the expansion in powers of $1/c^2$ of $E_{n,j} - mc^2$, where $E_{n,j}$ is the Dirac operator's eigenvalue given by Sommerfeld's celebrated *fine structure formula*

$$E_{n,j} \;=\; mc^2\Big(1 + \frac{(Z\alpha_{\mathrm{f}})^2}{(n - j - \frac{1}{2} + \sqrt{\kappa^2 - (Z\alpha_{\mathrm{f}})^2})^2}\Big)^{-\frac{1}{2}}. \tag{4.1.5}$$

Let us recall, in particular, the nature of the Darwin correction, which is induced by the interaction between the magnetic moment of the moving electron and the electric field $\mathbf{E} = \frac{1}{e}\nabla V$, where V is the potential energy due to the charge distribution that generates $\mathbf{E}$. This effect, to the first order in perturbation theory, produces an additive term to the non-relativistic Hamiltonian, which formally reads [12, §33]

$$H_{\mathrm{Darwin}} \;=\; -\frac{\hbar^2}{8m^2 c^2} e \operatorname{div}\mathbf{E} \;=\; -\frac{\hbar^2}{8m^2 c^2} \Delta V. \tag{4.1.6}$$

For a hydrogenoid atom $V(x) = -Ze^2/|x|$, whence $\Delta V = -4\pi Ze^2 \delta^{(3)}(x)$: the term (4.1.6) is therefore to be regarded as a *point-like perturbation* 'supported' at the centre of the atom, whose nuclear charge creates the field $\mathbf{E}$. In this case one gives meaning to (4.1.6) in the sense of the expectation

$$\langle\psi, H_{\mathrm{Darwin}}\psi\rangle \;=\; \frac{4\pi Ze^2\hbar^2}{8m^2 c^2} |\psi(0)|^2 \;=\; E_n^{(\mathrm{H})} \frac{(Z\alpha_{\mathrm{f}})^2}{n} \cdot \pi\Big(\frac{na_0}{Z}\Big)^3 |\psi(0)|^2, \tag{4.1.7}$$

where $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius.

Unlike the semi-relativistic kinetic energy and spin-orbit corrections, the Darwin correction only affects the s orbitals ($\ell = 0$, $j = \frac{1}{2}$), the wave functions of higher orbitals vanishing at $x = 0$. Since the s-wave normalised eigenfunction $\psi_n^{(\mathrm{H})}$ corresponding to $E_n^{(\mathrm{H})}$ satisfies $|\psi_n^{(\mathrm{H})}(0)|^2 = \frac{1}{\pi}(\frac{Z}{na_0})^3$, (4.1.7) implies

$$\left(\frac{\delta E_n^{(\mathrm{H})}}{E_n^{(\mathrm{H})}}\right)_{\mathrm{Darwin}} = \frac{(Z\alpha_{\mathrm{f}})^2}{n} \qquad (\ell = 0). \tag{4.1.8}$$

The above classical considerations are one of the typical motivations for the rigorous study of a 'simplified fine structure', low-energy correction of the ideal (non-relativistic) hydrogenoid Hamiltonian (4.1.1) that consists of a Darwin-like perturbation only. In particular, one considers an additional interaction that is only present in the s-wave sector.

This amounts to constructing self-adjoint Hamiltonians with Coulomb plus point interaction centred at the origin, and it requires to go beyond the formal perturbative arguments that yielded the spectral correction (4.1.8)

One natural approach, exploited first in the early 1980's works by Zorbas [126], by Albeverio, Gesztesy, Høegh-Krohn, and Streit [3], and by Bulla and Gesztesy [21], is to regard such Hamiltonians as self-adjoint extensions of the densely defined, symmetric, semi-bounded from below operator

$$\mathring{H}_{\mathrm{Hydr}} = \left(-\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{|x|}\right)\Big|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}. \tag{4.1.9}$$

For clarity of presentation we shall set $\nu := -Ze^2$, in fact allowing ν to be positive or negative real, and we shall work in units $2m = \hbar = e = 1$. We shall then write $H^{(\nu)}$ and $\mathring{H}^{(\nu)}$ for the operator $-\Delta + \frac{\nu}{|x|}$ defined, respectively, on the domain of self-adjointness $H^2(\mathbb{R}^3)$ or on the restriction domain $C_0^\infty(\mathbb{R}^3\setminus\{0\})$.

As was found in [126, 3, 21], the self-adjoint extensions of $\mathring{H}^{(\nu)}$ on $L^2(\mathbb{R}^3)$ at fixed ν form a one-parameter family $\{H_\alpha^{(\nu)}|\alpha \in (-\infty, +\infty]\}$ of rank-one perturbations, in the resolvent sense, of the Hamiltonian $H^{(\nu)}$. We state this famous result in Theorem 4.1.3 below.

In fact, in this chapter among other findings we shall *re-obtain* such a result through an alternative path. Indeed, the above-mentioned works [126, 3, 21] the standard self-adjoint extension theory a la von Neumann [118, Chapt. 8] was applied. We intend to exploit here an alternative construction and classification based on the Kreĭn-Višik-Birman extension scheme [51], owing to certain features of the latter theory that are somewhat more informative and cleaner, in the sense that we are going to specify in due time.

We also recall that the integral kernel of $(H^{(\nu)} - k^2\mathbb{1})^{-1}$ is explicitly known [65]:

$$(H^{(\nu)} - k^2\mathbb{1})^{-1}(x,y) = \Gamma(1 + \tfrac{\mathrm{i}\nu}{2k})\frac{\mathscr{A}_{\nu,k}(x,y)}{4\pi|x-y|}, \qquad x,y \in \mathbb{R}^3, \ x \neq y$$

$$\mathscr{A}_{\nu,k}(x,y) := \left(\frac{\mathrm{d}}{\mathrm{d}\xi} - \frac{\mathrm{d}}{\mathrm{d}\eta}\right)\mathscr{M}_{-\frac{\mathrm{i}\nu}{2k},\frac{1}{2}}(\xi)\,\mathscr{W}_{-\frac{\mathrm{i}\nu}{2k},\frac{1}{2}}(\eta)\Big|_{\substack{\xi=-\mathrm{i}kz_-\\\eta=-\mathrm{i}kz_+}} \tag{4.1.10}$$

$$z_\pm := |x| + |y| \pm |x-y|, \qquad k^2 \in \rho(H_\alpha^{(\nu)}), \quad \mathfrak{Im}\,k > 0,$$

where $\mathscr{M}_{a,b}$ and $\mathscr{W}_{a,b}$ are the Whittaker functions [1, Chapt. 13].

4.1.2 Angular decomposition

Let us exploit as customary the rotational symmetry of $H^{(\nu)}$ and $\mathring{H}^{(\nu)}$ by passing to polar coordinates $x \equiv (r, \Omega) \in \mathbb{R}^+ \times \mathbb{S}^2$, $r := |x|$, for $x \in \mathbb{R}^3$. This induces the standard isomorphism

$$
\begin{aligned}
L^2(\mathbb{R}^3, \mathrm{d}x) &\cong U^{-1} L^2(\mathbb{R}^+, \mathrm{d}r) \otimes L^2(\mathbb{S}^2, \mathrm{d}\Omega) \\
&\cong \bigoplus_{\ell=0}^{\infty} \Big(U^{-1} L^2(\mathbb{R}^+, \mathrm{d}r) \otimes \mathrm{span}\{Y_\ell^{-\ell}, \dots, Y_\ell^\ell\} \Big)
\end{aligned}
\tag{4.1.11}
$$

where $U : L^2(\mathbb{R}^+, r^2 \mathrm{d}r) \to L^2(\mathbb{R}^+, \mathrm{d}r)$ is the unitary $(Uf)(r) = r f(r)$, and the Y_ℓ^m's are the spherical harmonics on $\mathbb{S}^2$, i.e., the common eigenfunctions of $\boldsymbol{L}^2$ and $\boldsymbol{L}_3$ of eigenvalue $\ell(\ell+1)$ and m respectively, $\boldsymbol{L} = x \times (-\mathrm{i}\nabla)$ being the angular momentum operator.

Standard arguments show that $\mathring{H}^{(\nu)}$ (and analogously $H^{(\nu)}$) is reduced by the decomposition (4.1.11) as

$$
\mathring{H}^{(\nu)} \cong \bigoplus_{\ell=0}^{\infty} \Big(U^{-1} h_\ell^{(\nu)} U \otimes \mathbb{1} \Big)
\tag{4.1.12}
$$

where each $h_\ell^{(\nu)}$ is the operator on $L^2(\mathbb{R}^+, \mathrm{d}r)$ defined by

$$
h_\ell^{(\nu)} := -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2} + \frac{\nu}{r}, \qquad \mathcal{D}\big(h_\ell^{(\nu)}\big) := C_0^\infty(\mathbb{R}^+).
\tag{4.1.13}
$$

4.1.3   The radial problem

Owing to (4.1.11)-(4.1.12), the question of the self-adjoint extensions of $\mathring{H}^{(\nu)}$ on $L^2(\mathbb{R}^3, \mathrm{d}x)$ is the same as the question of the self-adjoint extensions of each $h_\ell^{(\nu)}$ on $L^2(\mathbb{R}^+)$.

Based on the classical analysis of Weyl (see Section 1.4), all the block operators $h_\ell^{(\nu)}$ with $\ell \in \mathbb{N}$ are essentially self-adjoint, as they are both in the limit point case at infinity (Proposition 1.4.4) and in the limit point case at zero (Proposition 1.4.5).

One could also add (but we shall retrieve this conclusion along a different path) that $h_0^{(\nu)}$ is still in the limit point case at infinity, yet limit circle at zero [104, Prop. 15.12(ii)], thus, admitting a one-parameter family of self-adjoint extensions [104, Theorem 15.10(ii)].

We notice that, according to this preliminary analysis, we are in condition to apply Theorem 3.2.22 which ensures that all self-adjoint extensions of the operator (4.1.9) preserve the invariance under rotations.

The question of the self-adjoint realisations of $\mathring{H}^{(\nu)}$ is then boiled down to the self-adjointness problem for $h_0^{(\nu)}$ on $L^2(\mathbb{R}^+)$.

This too is a problem studied since long, that we want to re-consider from an alternative, instructive perspective.

The novelty of the present analysis, as we shall see, besides the explicit qualification of the closure and of the Friedrichs extension of $h_0^{(\nu)}$, is the relatively straightforward application of the alternative extension scheme of Kreĭn, Višik, and Birman.

4.1.4   Main results

Let us finally come to the main results of this chapter. On the one hand, as mentioned already, we reproduce classical facts (namely Theorem 4.1.2 for the radial problem and Theorem 4.1.3 for the singularly-perturbed hydrogenoid Hamiltonians) through the alternative extension scheme of Kreĭn, Višik, and Birman. On the other hand, we qualify previously studied objects in an explicit, new form, specifically the Friedrichs realisation of the radial operator (Theorem 4.1.1) and our final formula for the central perturbation of the hydrogenoid spectra (Theorem 4.1.4).

Clearly, whereas the derivatives in (4.1.9) and (4.1.13) are *classical*, the following formulas contain *weak* derivatives.

As a first step, we identify the closure and the Friedrichs realisation of the radial problem.

Theorem 4.1.1 (Closure and Friedrichs extension of $h_0^{(\nu)}$)**.**
The operator $h_0^{(\nu)}$ is semi-bounded from below with deficiency index one.

(i) *One has*

$$
\begin{aligned}
\mathcal{D}(\overline{h_0^{(\nu)}}) &= H_0^2(\mathbb{R}^+) = \overline{C_0^\infty(\mathbb{R}^+)}^{\| \,\|_{H^2}} \\
\overline{h_0^{(\nu)}} f &= -f'' + \frac{\nu}{r} f \,.
\end{aligned}
\tag{4.1.14}
$$

The Friedrichs extension $h_{0,F}^{(\nu)}$ of $h_0^{(\nu)}$ has

(ii) *operator domain and action given by*

$$
\begin{aligned}
\mathcal{D}(h_{0,F}^{(\nu)}) &= H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+) = \{f \in H^2(\mathbb{R}^+) \,|\, \lim_{r\downarrow 0} f(r) = 0\} \\
h_{0,F}^{(\nu)} f &= -f'' + \frac{\nu}{r} f \,;
\end{aligned}
\tag{4.1.15}
$$

(iii) *quadratic form given by*

$$
\begin{aligned}
\mathcal{D}[h_{0,F}] &= H_0^1(\mathbb{R}^+) \\
h_{0,F}^{(\nu)}[f,h] &= \int_0^{+\infty} \left(\overline{f'(r)} h'(r) + \nu \frac{\overline{f(r)}h(r)}{r} \right) \mathrm{d}r \,;
\end{aligned}
\tag{4.1.16}
$$

(iv) *resolvent with integral kernel*

$$
\left(h_{0,F}^{(\nu)} + \frac{\nu^2}{4\kappa^2} \right)^{-1}(r,\rho) = -\frac{\kappa\Gamma(1-\kappa)}{\nu}
\begin{cases}
\mathscr{W}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa}r)\mathscr{M}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa}\rho) & \text{if } 0 < \rho < r \\
\mathscr{M}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa}r)\mathscr{W}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa}\rho) & \text{if } 0 < r < \rho,
\end{cases}
\tag{4.1.17}
$$

where $\kappa \in (-\infty,0)\cup(0,1)$, $\mathrm{sign}\,\kappa = -\mathrm{sign}\,\nu$, and where $\mathscr{W}_{a,b}(r)$ and $\mathscr{M}_{a,b}(r)$ are the Whittaker functions.

Next, using the Friedrichs extension as a *reference extension* for the Kreĭn-Višik-Birman scheme, we classify all other self-adjoint realisations of the radial problem. The result is classical in the literature [98, 21], but we find the present derivation more straightforward and natural, especially in yielding the typical boundary condition at the origin that qualify each extension.

Theorem 4.1.2 (Self-adjoint realisations of $h_0^{(\nu)}$)**.**

(i) *The self-adjoint extensions of $h_0^{(\nu)}$ form the family $(h_{0,\alpha}^{(\nu)})_{\alpha\in\mathbb{R}\cup\{\infty\}}$, where $\alpha = \infty$ labels the Friedrichs extension, and*

$$
\begin{aligned}
\mathcal{D}(h_{0,\alpha}^{(\nu)}) &= \left\{ g \in L^2(\mathbb{R}^+) \,\middle|\, \begin{array}{c} -g'' + \frac{\nu}{r}g \in L^2(\mathbb{R}^+) \\ \text{and } g_1 = 4\pi\alpha\, g_0 \end{array} \right\} \\
h_{0,\alpha}^{(\nu)} g &= -g'' + \frac{\nu}{r} g \,,
\end{aligned}
\tag{4.1.18}
$$

g_0 *and* g_1 *being the existing limits*

$$
\begin{aligned}
g_0 &:= \lim_{r\downarrow 0} g(r) \\
g_1 &:= \lim_{r\downarrow 0} r^{-1}\big(g(r) - g_0(1 + \nu r \ln r)\big) \,.
\end{aligned}
\tag{4.1.19}
$$

(ii) For given $\kappa \in (-\infty, 0) \cup (0, 1)$, $\operatorname{sign} \kappa = -\operatorname{sign} \nu$, one has

$$\left(h_{0,\alpha}^{(\nu)} + \frac{\nu^2}{4\kappa^2} \right)^{-1} = \left(h_{0,\infty}^{(\nu)} + \frac{\nu^2}{4\kappa^2} \right)^{-1} + \frac{\Gamma(1-\kappa)^2}{4\pi} \frac{1}{\alpha - \mathfrak{F}_{\nu,\kappa}} |\Phi_\kappa\rangle\langle\Phi_\kappa| , \tag{4.1.20}$$

where $\Phi_\kappa(r) := \mathscr{W}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa} r)$ and

$$\mathfrak{F}_{\nu,\kappa} := \frac{\nu}{4\pi} \left(\psi(1-\kappa) + \ln(-\tfrac{\nu}{\kappa}) + (2\gamma - 1) + \tfrac{1}{2\kappa} \right). \tag{4.1.21}$$

Consistently, when $\nu = 0$ the boundary condition (4.1.18) for the α-extension takes the classical form $g'(0) = 4\pi\alpha g(0)$, namely the well-known boundary condition for the generic self-adjoint Laplacian on the half-line [73, 55, 34].

When the radial analysis is lifted back to the three-dimensional Hilbert space, we re-obtain, through an alternative path, the following classification result already available in the literature (see, e.g., [4, Theorem I.2.1.2]).

Theorem 4.1.3 (Self-adjoint realisations of $\mathring{H}^{(\nu)}$).
The self-adjoint extensions of $\mathring{H}^{(\nu)}$ form the family $(H_\alpha^{(\nu)})_{\alpha \in \mathbb{R} \cup \{\infty\}}$ characterised as follows.

(i) With respect to the canonical decomposition (4.1.11) of $L^2(\mathbb{R}^3)$, the extension $H_\alpha^{(\nu)}$ is reduced as

$$H_\alpha^{(\nu)} \cong \bigoplus_{\ell=0}^{\infty} \left(U^{-1} h_{\ell,\alpha}^{(\nu)} U \otimes \mathbb{1} \right), \tag{4.1.22}$$

where $h_{0,\alpha}^{(\nu)}$ is qualified in Theorem 4.1.2 and $h_{\ell,\alpha}^{(\nu)}$, for $\ell \geqslant 1$, is the closure of $h_\ell^{(\nu)}$ introduced in (4.1.13), namely the $L^2(\mathbb{R}^+)$-self-adjoint operator

$$\begin{aligned} \mathcal{D}(h_{\ell,\alpha}^{(\nu)}) &= \{ g \in L^2(\mathbb{R}^+) \,|\, -g'' + \tfrac{\ell(\ell+1)}{r^2} g + \tfrac{\nu}{r} g \in L^2(\mathbb{R}^+) \} \\ h_{\ell,\alpha}^{(\nu)} g &= -g'' + \tfrac{\ell(\ell+1)}{r^2} g + \tfrac{\nu}{r} g \,. \end{aligned} \tag{4.1.23}$$

(ii) The choice $\alpha = \infty$ identifies the Friedrichs extension of $\mathring{H}^{(\nu)}$, which is precisely the self-adjoint hydrogenoid Hamiltonian

$$H^{(\nu)} = -\Delta + \frac{\nu}{|x|}, \qquad \mathcal{D}(H^{(\nu)}) = H^2(\mathbb{R}^3). \tag{4.1.24}$$

It is the only member of the family $(H_\alpha^{(\nu)})_{\alpha \in \mathbb{R} \cup \{\infty\}}$ whose domain's functions have separately finite kinetic and finite potential energy, in the sense of energy forms.

(iii) For given $\kappa \in (-\infty, 0) \cup (0, 1)$, $\operatorname{sign} \kappa = -\operatorname{sign} \nu$, one has

$$\left(H_\alpha^{(\nu)} + \frac{\nu^2}{4\kappa^2} \mathbb{1} \right)^{-1} = \left(H^{(\nu)} + \frac{\nu^2}{4\kappa^2} \mathbb{1} \right)^{-1} + \frac{1}{\alpha - \mathfrak{F}_{\nu,\kappa}} |\mathfrak{g}_{\nu,\kappa}\rangle\langle\mathfrak{g}_{\nu,\kappa}| , \tag{4.1.25}$$

where

$$\mathfrak{g}_{\nu,\kappa}(x) := \Gamma(1-\kappa) \frac{\mathscr{W}_{\kappa,\frac{1}{2}}(-\frac{\nu}{\kappa}|x|)}{4\pi|x|} \tag{4.1.26}$$

and $\mathfrak{F}_{\nu,\kappa}$ is defined in (4.1.21).

(iv) For given $\kappa \in (-\infty, 0) \cup (0, 1)$, $\operatorname{sign} \kappa = -\operatorname{sign} \nu$, one has

$$\mathcal{D}(H_\alpha^{(\nu)}) = \left\{ \psi = \varphi_\kappa + \frac{\varphi_\kappa(0)}{\alpha - \mathfrak{F}_{\nu,\kappa}} \mathfrak{g}_{\nu,\kappa} \,\Big|\, \varphi_\kappa \in H^2(\mathbb{R}^3) \right\}$$

$$\left(H_\alpha^{(\nu)} + \frac{\nu^2}{4\kappa^2} \mathbb{1} \right) \psi = \left(H^{(\nu)} + \frac{\nu^2}{4\kappa^2} \mathbb{1} \right) \varphi_\kappa ,$$

(4.1.27)

the decomposition of each ψ being unique.

We observe that (4.1.27) provides the typical decomposition of a generic element in $\mathcal{D}(H_\alpha^{(\nu)})$ into the 'regular' part $\varphi_\kappa \in H^2(\mathbb{R}^3)$ and the 'singular' part $\mathfrak{g}_{\nu,\kappa} \sim |x|^{-1}$ as $x \to 0$ with a precise 'boundary condition' among the two.

The uniqueness property of part (ii) above is another feature that, as we shall see, emerges naturally within the Kreĭn-Višik-Birman scheme. It gives the standard hydrogenoid Hamiltonian a somewhat physically distinguished status, in complete analogy with its semi-relativistic counterpart, the well-known distinguished realisation of the Dirac-Coulomb Hamiltonian (see, e.g., [47, 50] and the references therein).

Last, we address the spectral analysis of each realisation $H_\alpha^{(\nu)}$.

Since the $H_\alpha^{(\nu)}$'s are rank-one perturbations, in the resolvent sense, of $H_{\alpha=\infty}^{(\nu)} \equiv H^{(\nu)}$, then we deduce from (4.1.2) that

$$\sigma_{\mathrm{ess}}(H_\alpha^{(\nu)}) = \sigma_{\mathrm{ac}}(H_\alpha^{(\nu)}) = [0, +\infty), \quad \sigma_{\mathrm{sc}}(H_\alpha^{(\nu)}) = \varnothing ,$$

(4.1.28)

and only $\sigma_{\mathrm{point}}(H_\alpha^{(\nu)})$ differs from the corresponding $\sigma_{\mathrm{point}}(H^{(\nu)})$.

Concerning the corrections to $\sigma_{\mathrm{point}}(H^{(\nu)})$ due to the central perturbation, we distinguish among the two possible cases. If $\nu < 0$, then the n-th eigenvalue $-\frac{\nu^2}{4n^2}$ in $\sigma_{\mathrm{point}}(H^{(\nu)})$ is n^2-fold degenerate, with partial $(2\ell + 1)$-fold degeneracy in the sector of angular symmetry ℓ for all $\ell \in \{0, \dots, n-1\}$. All the eigenstates of $H^{(\nu)}$ with eigenvalue $-\frac{\nu^2}{4n^2}$ and with symmetry $\ell \geqslant 1$ are also eigenstates of any other realisation $H_\alpha^{(\nu)}$ with the same eigenvalue, because $H_\alpha^{(\nu)}$ is a perturbation of $H^{(\nu)}$ in the s-wave only. Thus, the effect of the central perturbation is a correction to the $\ell = 0$ point spectrum of $H^{(\nu)}$, which consists of countably many non-degenerate eigenvalues $E_n := -\frac{\nu^2}{4n^2}$, $n \in \mathbb{N}$.

If instead $\nu > 0$, then a standard application of the Kato-Agmon-Simon Theorem (see e.g. [96, Theorem XIII.58]) gives $\sigma_{\mathrm{point}}(H^{(\nu)}) = \varnothing$. Yet, if the central perturbation corresponds to an interaction that is attractive or at least not too much repulsive, then it can create one negative eigenvalue in the $\ell = 0$ sector.

This is described in detail as follows.

Theorem 4.1.4 (Eigenvalue corrections).
For given $\alpha \in \mathbb{R} \cup \{\infty\}$ and $\nu \in \mathbb{R}$, let $\sigma_{\mathrm{p}}^{(0)}(H_\alpha^{(\nu)})$ be point spectrum of the self-adjoint extension $H_\alpha^{(\nu)}$ with definite angular symmetry $\ell = 0$ ('s-wave point spectrum'). Moreover, for $E < 0$ let

$$\mathfrak{F}_\nu(E) := \frac{\nu}{4\pi} \left(\psi \big(1 + \tfrac{\nu}{2\sqrt{|E|}} \big) + \ln(2\sqrt{|E|}) + 2\gamma - 1 - \frac{\sqrt{|E|}}{\nu} \right).$$

(4.1.29)

(i) If $\nu < 0$, then the equation

$$\mathfrak{F}_\nu(E) = \alpha$$

(4.1.30)

admits countably many simple negative roots that form an increasing sequence $(E_n^{(\nu,\alpha)})_{n\in\mathbb{N}}$ accumulating at zero, and

$$\sigma_{\mathrm{p}}^{(0)}(H_\alpha^{(\nu)}) = \left\{ E_n^{(\nu,\alpha=\infty)} \,\big|\, n \in \mathbb{N} \right\}.$$
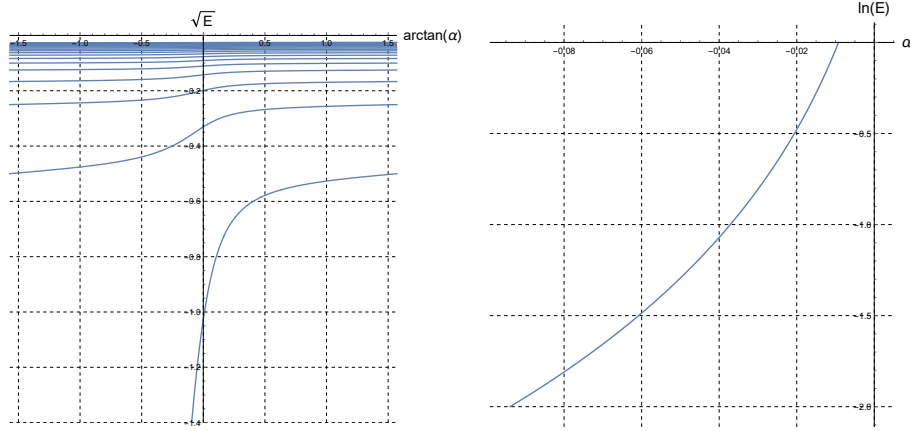
(4.1.31)

Figure 4.1: Eigenvalues of the perturbed hydrogenoid Hamiltonian $H_\alpha^{(\nu)}$ for $\nu = -1$ (left) and $\nu = 1$ (right). The scales of the energy E and of the extension parameter α are modified to magnify the behaviour of the eigenvalues.

For the Friedrichs extension,

$$E_n^{(\nu,\alpha=\infty)} \;=\; E_n^{(\nu)} \;=\; -\frac{\nu^2}{4n^2}\,, \tag{4.1.32}$$

that is, the ordinary hydrogenoid eigenvalues.

(ii) If $\nu > 0$, then the equation (4.1.30) has no negative roots if $\alpha \geqslant \alpha_\nu$, where

$$\alpha_\nu \;:=\; \frac{\nu}{4\pi}\,(\ln\nu + 2\gamma - 1)\,, \tag{4.1.33}$$

and has one simple negative root $E_+^{(\nu,\alpha)}$ if $\alpha < \alpha_\nu$. Correspondingly,

$$\sigma_{\mathrm{p}}^{(0)}(H_\alpha^{(\nu)}) \;=\; \begin{cases} \varnothing & if\ \alpha \geqslant \alpha_\nu\,, \\ E_+^{(\nu,\alpha)} & if\ \alpha < \alpha_\nu\,. \end{cases} \tag{4.1.34}$$

Figure 4.1 displays the structure of the discrete spectrum described in Theorem 4.1.4 above.

As we shall argue rigorously in due time, Figure 4.1 confirms that when $\nu < 0$ each $E_n^{(\nu,\alpha)}$ is smooth and strictly monotone in α, with a typical *fibred structure* of the union of all the discrete spectra $\sigma_{\mathrm{disc}}(H_\alpha^{(\nu)})$

$$(-\infty, 0) \;=\; \bigcup_{\alpha\in(-\infty,+\infty]} \{E_n^{(\nu,\alpha)} \,|\, n \in \mathbb{N}\} \;=\; \mathbb{R} \setminus \sigma_{\mathrm{ess}}(H_\alpha^{(\nu)})\,, \tag{4.1.35}$$

(see Remark 4.3.2 below, and Theorem 5.1.32 for an analogous phenomenon for Dirac operators), and the correction $E_n^{(\nu,\alpha)}$ to the non-relativistic $E_n^{(\nu)}$ always *decreases* the energy, with the intertwined relation $E_{n+1}^{(\nu,\alpha)} \geqslant E_n^{(\nu)} \geqslant E_n^{(\nu,\alpha)}$ (see Remark 4.3.1).

Analogously, when $\nu > 0$,

$$(-\infty, 0) \;=\; \bigcup_{\alpha\in(-\infty,\alpha_\nu)} \{E_+^{(\nu,\alpha)}\} \;=\; \mathbb{R} \setminus \sigma_{\mathrm{ess}}(H_\alpha^{(\nu)})\,. \tag{4.1.36}$$

4.2 Self-adjoint realisations and classification

In this Section we establish the constructions of Theorems 4.1.1, 4.1.2, and 4.1.3. The main focus are the self-adjoint extensions on $L^2(\mathbb{R}^+)$ of the radial operator $h_0^{(\nu)}$. Equivalently, we study the self-adjoint extensions of the shifted operator

$$S := -\frac{d^2}{dr^2} + \frac{\nu}{r} + \frac{\nu^2}{4\kappa^2}, \qquad \mathcal{D}(S) := C_0^\infty(\mathbb{R}^+), \tag{4.2.1}$$

for generic

$$\kappa \in \mathbb{R}, \qquad \operatorname{sign}\kappa = -\operatorname{sign}\nu, \qquad 0 < |\kappa| < \tfrac{1}{2}. \tag{4.2.2}$$

Owing to (4.1.2), $-\frac{d^2}{dr^2} + \frac{\nu}{r} \geqslant -\nu^2/4$, whence $S \geqslant \frac{1}{4}\nu^2(\kappa^{-2} - 1)$: thus, S is densely defined and symmetric on $L^2(\mathbb{R}^+)$ with *strictly positive bottom*. This feature will simplify the identification of the self-adjoint extensions of S: the corresponding extensions for $h_0^{(\nu)}$ are then obtained through a trivial shift.

It will be also convenient to make use of the notation

$$\widetilde{S} := -\frac{d^2}{dr^2} + \frac{\nu}{r} + \frac{\nu^2}{4\kappa^2} \tag{4.2.3}$$

to refer to the *differential* action on functions in $L^2(\mathbb{R}^+)$, in the classical or the weak sense, with no reference to the operator domain.

In order to apply the Kreĭn-Višik-Birman extension scheme of Chapter 2, an amount of preparatory steps are needed (Subsect. 4.2.1 through 4.2.4), in which we identify the spaces $\mathcal{D}(\overline{S})$, $\ker S^*$, and $S_F^{-1} \ker S^*$, S_F being the Friedrichs extension of S. In Subsect. 4.2.4 we qualify S_F and prove Theorem 4.1.1; in Subsect. 4.2.5 we classify the extensions of S and prove Theorem 4.1.2; last, in Subsect. 4.2.6 we deduce Theorem 4.1.3 from the previous results.

4.2.1 The homogeneous radial problem

We first qualify the space $\ker S^*$. By standard arguments (see, e.g., [104, Lemma 15.1])

$$\mathcal{D}(S^*) = \left\{ g \in L^2(\mathbb{R}^+) \,\middle|\, \widetilde{S}g \in L^2(\mathbb{R}^+) \right\}$$

$$S^*g = \widetilde{S}g = -g'' + \frac{\nu}{r}g + \frac{\nu^2}{4\kappa^2}g, \tag{4.2.4}$$

that is, S^* is the *maximal* realisation of $\widetilde{S}$, and in fact $\overline{S}$ is the *minimal* one. Thus, $\ker S^*$ is formed by the square-integrable solutions to $\widetilde{S}u = 0$ on $\mathbb{R}^+$. It is also standard (see e.g. [116, Theorems 5.2–5.4]) that if u solves $\widetilde{S}u = 0$, then it is smooth on $\mathbb{R}^+$, with possible singularity only at zero or infinity.

Through the change of variable $\rho := -\frac{\nu}{\kappa}r$, $w(\rho) := u(r)$, where $-\frac{\nu}{\kappa} > 0$ for every non-zero ν owing to (4.2.2), the differential problem becomes

$$\left(-\frac{d^2}{d\rho^2} - \frac{\kappa}{\rho} + \frac{1}{4} \right) w = 0, \tag{4.2.5}$$

that is, a special case of Whittaker's equation $w'' - (\frac{1}{4} - \frac{\kappa}{\rho} + (\frac{1}{4} - \mu^2)\frac{1}{\rho^2})w = 0$ with parameter $\mu = \frac{1}{2}$ [1, Eq. (13.1.31)]. The functions

$$\mathscr{M}_{\kappa,\frac{1}{2}}(\rho) = e^{-\frac{1}{2}\rho}\rho\, M_{1-\kappa,2}(\rho) \tag{4.2.6}$$

$$\mathscr{W}_{\kappa,\frac{1}{2}}(\rho) = e^{-\frac{1}{2}\rho}\rho\, U_{1-\kappa,2}(\rho) \tag{4.2.7}$$

form a pair $(\mathscr{M}_{\kappa,\frac{1}{2}}, \mathscr{W}_{\kappa,\frac{1}{2}})$ of linearly independent solutions to (4.2.5) [1, Eq. (13.1.32)-(13.1.33)], where $M_{a,b}$ and $U_{a,b}$ are, respectively, Kummer's and Tricomi's function [1, Eq. (13.1.2)-(13.1.3)].

Owing to [1, Eq. (13.5.5), (13.5.7), (13.1.2) and (13.1.6)] as $\rho \to 0$, and to [1, Eq. (13.1.4) and (13.1.8)] as $\rho \to +\infty$, one has the asymptotics

$$\mathscr{M}_{\kappa,\frac{1}{2}}(\rho) \overset{\rho\to 0}{=} \rho - \frac{\kappa}{2}\rho^2 + \frac{1+2\kappa^2}{24}\rho^3 + O(\rho^4)$$

$$\mathscr{W}_{\kappa,\frac{1}{2}}(\rho) \overset{\rho\to 0}{=} \frac{1}{\Gamma(1-\kappa)} - \frac{\kappa}{\Gamma(1-\kappa)}\rho \ln\rho$$

$$+ \frac{(2-4\gamma)\kappa - 2\kappa\psi(1-\kappa) - 1}{2\Gamma(1-\kappa)}\rho + O(\rho^2\ln\rho) \tag{4.2.8}$$

and

$$\mathscr{M}_{\kappa,\frac{1}{2}}(\rho) \overset{\rho\to +\infty}{=} \frac{1}{\Gamma(1-\kappa)}e^{\rho/2}\rho^{-\kappa}(1+O(\rho^{-1}))$$

$$\mathscr{W}_{\kappa,\frac{1}{2}}(\rho) \overset{\rho\to +\infty}{=} e^{-\rho/2}\rho^{\kappa}(1+O(\rho^{-1})), \tag{4.2.9}$$

where $\gamma \sim 0.577$ is the Euler-Mascheroni constant and $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the digamma function. Since $0 < |\kappa| < \frac{1}{2}$, the expressions (4.2.8) and (4.2.9) make sense.

Therefore only $\mathscr{W}_{\kappa,\frac{1}{2}}$ is square-integrable at infinity, whereas both $\mathscr{M}_{\kappa,\frac{1}{2}}$ and $\mathscr{W}_{\kappa,\frac{1}{2}}$ are square-integrable at zero. This implies that the square-integrable solutions to $\widetilde{S}u = 0$ form a *one-dimensional* space, that is, $\dim \ker S^* = 1$.

Explicitly, upon setting

$$F_\kappa(r) := \mathscr{M}_{\kappa,\frac{1}{2}}(\lambda r)$$

$$\Phi_\kappa(r) := \mathscr{W}_{\kappa,\frac{1}{2}}(\lambda r), \qquad \lambda := -\frac{\nu}{\kappa} > 0, \tag{4.2.10}$$

one has that

$$\ker S^* = \mathrm{span}\{\Phi_\kappa\} \tag{4.2.11}$$

and that (F_κ, Φ_κ) is a pair of linearly independent solutions to the original problem $\widetilde{S}u = 0$.

4.2.2   Inhomogeneous inverse radial problem

Next, let us focus on the inhomogeneous problem $\widetilde{S}f = g$ in the unknown f for given g. With respect to the fundamental system (F_κ, Φ_κ) for $\widetilde{S}u = 0$, the general solution is given by

$$f = c_1 F_\kappa + c_2 \Phi_\kappa + f_{\mathrm{part}} \tag{4.2.12}$$

for $c_1, c_2 \in \mathbb{C}$ and some particular solution f_{part}, i.e., $\widetilde{S}f_{\mathrm{part}} = g$.

The Wronskian

$$W(\Phi_\kappa, F_\kappa)(r) := \det\begin{pmatrix} \Phi_\kappa(r) & F_\kappa(r) \\ \Phi_\kappa'(r) & F_\kappa'(r) \end{pmatrix} \tag{4.2.13}$$

relative to the pair (F_κ, Φ_κ) is actually constant in r, owing to Liouville's theorem, with a value that can be computed by means of the asymptotics (4.2.8) or (4.2.9) and amounts to

$$W(\Phi_\kappa, F_\kappa) = \frac{-\nu/\kappa}{\Gamma(1-\kappa)} =: W. \tag{4.2.14}$$

A standard application of the method of variation of constants [116, Section 2.4] shows that we can take f_{part} to be

$$f_{\text{part}}(r) \;=\; \int_0^{+\infty} G(r,\rho)g(\rho)\,\mathrm{d}\rho\,, \tag{4.2.15}$$

where

$$G(r,\rho) \;:=\; \frac{1}{W} \begin{cases} \Phi_\kappa(r)F_\kappa(\rho) & \text{if } 0 < \rho < r \\ F_\kappa(r)\Phi_\kappa(\rho) & \text{if } 0 < r < \rho\,. \end{cases} \tag{4.2.16}$$

The following property holds.

Lemma 4.2.1. *The integral operator R_G on $L^2(\mathbb{R}^+, \mathrm{d}r)$ with kernel $G(r,\rho)$ given by (4.2.16) is bounded and self-adjoint.*

Proof. R_G splits into the sum of four integral operators with kernels given by

$$\begin{aligned} G^{++}(r,\rho) &:= G(r,\rho)\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \\ G^{+-}(r,\rho) &:= G(r,\rho)\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(0,1)}(\rho) \\ G^{-+}(r,\rho) &:= G(r,\rho)\,\mathbf{1}_{(0,1)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \\ G^{--}(r,\rho) &:= G(r,\rho)\,\mathbf{1}_{(0,1)}(r)\,\mathbf{1}_{(0,1)}(\rho)\,, \end{aligned}$$

where $\mathbf{1}_J$ denotes the characteristic function of the interval $J \subset \mathbb{R}^+$. We can estimate each $G^{LM}(r,\rho)$, $L, M \in \{+, -\}$, by means of the short and large distance asymptotics (4.2.8)-(4.2.9) for F_κ and Φ_κ. Calling $\lambda = -\frac{\nu}{\kappa}$ as in (4.2.10), for example,

$$\left| \Phi_\kappa(r)\,F_\kappa(\rho)\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \right| \;\lesssim\; e^{-\frac{\lambda}{2}(r-\rho)} \left(\frac{r}{\rho} \right)^\kappa \qquad \text{if } 0 < \rho < r$$

$$\left| F_\kappa(r)\,\Phi_\kappa(\rho)\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \right| \;\lesssim\; e^{-\frac{\lambda}{2}(\rho-r)} \left(\frac{\rho}{r} \right)^\kappa \qquad \text{if } 0 < r < \rho\,,$$

because F_k diverges exponentially and Φ_κ vanishes exponentially as $r \to +\infty$. Thus,

$$\left| G^{++}(r,\rho) \right| \;\lesssim\; e^{-\frac{\lambda}{4}|r-\rho|}\,.$$

With analogous reasoning we find

$$\begin{aligned} \left| G^{++}(r,\rho) \right| &\lesssim e^{-\frac{\lambda}{4}|r-\rho|}\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \\ \left| G^{+-}(r,\rho) \right| &\lesssim e^{-\frac{\lambda}{4}r}\,\mathbf{1}_{(1,+\infty)}(r)\,\mathbf{1}_{(0,1)}(\rho) \\ \left| G^{-+}(r,\rho) \right| &\lesssim e^{-\frac{\lambda}{4}\rho}\,\mathbf{1}_{(0,1)}(r)\,\mathbf{1}_{(1,+\infty)}(\rho) \\ \left| G^{--}(r,\rho) \right| &\lesssim \mathbf{1}_{(0,1)}(r)\,\mathbf{1}_{(0,1)}(\rho)\,. \end{aligned} \tag{*}$$

The last three bounds in (*) imply $G^{+-}, G^{-+}, G^{--} \in L^2(\mathbb{R}^+ \times \mathbb{R}^+, \mathrm{d}r\,\mathrm{d}\rho)$ and therefore the corresponding integral operators are Hilbert-Schmidt operators on $L^2(\mathbb{R}^+)$. The first bound in (*) allows to conclude, by an obvious Schur test, that also the integral operator with kernel $G^{++}(r,\rho)$ is bounded on $L^2(\mathbb{R}^+)$. This proves the overall boundedness of R_G. Its self-adjointness is then clear from (4.2.16): the adjoint R_G^* of R_G has kernel $\overline{G(\rho, r)}$, but G is real-valued and $G(\rho, r) = G(r, \rho)$, thus proving that $R_G^* = R_G$. $\square$

4.2.3 Distinguished extension and its inverse

In the Kreĭn-Višik-Birman scheme one needs a *reference* self-adjoint extension of S with everywhere defined bounded inverse: the Friedrichs extension S_F is surely so, since the bottom of S is strictly positive by construction.

In this Subsection we shall prove the following.

Proposition 4.2.2. $R_G = S_F^{-1}$.

This is checked in several steps. First, we recognise that R_G inverts a self-adjoint extension of S.

Lemma 4.2.3. *There exists a self-adjoint extension $\mathscr{S}$ of S in $L^2(\mathbb{R}^+)$ which has everywhere defined and bounded inverse and such that $\mathscr{S}^{-1} = R_G$.*

Proof. R_G is bounded and self-adjoint (Lemma 4.2.1), and by construction satisfies $\widetilde{S} R_G g = g$ $\forall g \in L^2(\mathbb{R}^+)$. Therefore, $R_G g = 0$ for some $g \in L^2(\mathbb{R}^+)$ implies $g = 0$, i.e., R_G is injective. Then R_G has dense range $((\operatorname{ran} R_G)^\perp = \ker R_G)$. As such (see, e.g., [104, Theorem 1.8(iv)]), $\mathscr{S} := R_G^{-1}$ is self-adjoint. One thus has $R_G = \mathscr{S}^{-1}$ and from the identity $S^* R_G = \mathbb{1}$ on $L^2(\mathbb{R}^+)$ one deduces that for any $f \in \mathcal{D}(\mathscr{S})$, say, $f = R_G g = \mathscr{S}^{-1} g$ for some $g \in L^2(\mathbb{R}^+)$, the identity $S^* f = \mathscr{S} f$ holds. This means that $S^* \supset \mathscr{S}$, whence also $\overline{S} = S^{**} \subset \mathscr{S}$, i.e., $\mathscr{S}$ is a self-adjoint extension of S. $\qquad\square$

Next, we recall the following concerning the form of the Friedrichs extension. Let us define

$$\|f\|_F^2 \ := \ \langle f, Sf \rangle + \langle f, f \rangle, \tag{4.2.17}$$

which, for $f \in C_0^\infty(\mathbb{R}^+)$, is a norm equal to

$$\|f\|_F^2 \ = \ \|f'\|_{L^2}^2 + \nu \|r^{-\frac{1}{2}}f\|_{L^2}^2 + (\tfrac{\nu^2}{4\,\kappa^2} + 1)\|f\|_{L^2}^2. \tag{4.2.18}$$

Lemma 4.2.4. *The quadratic form of the Friedrichs extension of S is given by*

$$\begin{aligned}
\mathcal{D}[S_F] \ &= \ \big\{ f \in L^2(\mathbb{R}^+) \,\big|\, \|f'\|_{L^2}^2 + \nu \|r^{-\frac{1}{2}}f\|_{L^2}^2 + \|f\|_{L^2}^2 < +\infty \big\} \\
S_F[f,h] \ &= \ \int_0^{+\infty} \Big(\overline{f'(r)}h'(r) + \nu \,\frac{\overline{f(r)}h(r)}{r} + \frac{\nu^2}{4\,\kappa^2}\,\overline{f(r)}h(r) \Big)\mathrm{d}r\,.
\end{aligned} \tag{4.2.19}$$

Proof. A standard construction (see, e.g., Theorem 1.3.2), that follows from the fact that $\mathcal{D}[S_F]$ is the closure of $\mathcal{D}(S) = C_0^\infty(\mathbb{R}^+)$ in the norm $\|\cdot\|_F$: then (4.2.19) follows at once from (4.2.17)-(4.2.18). $\qquad\square$

In fact, the Friedrichs form domain is a classical functional space.

Lemma 4.2.5. $\mathcal{D}[S_F] \ = \ H_0^1(\mathbb{R}^+) := \overline{C_0^\infty(\mathbb{R}^+)}^{\|\ \|_{H^1}}$.

Proof. Hardy's inequality

$$\|r^{-1}f\|_{L^2} \ \leqslant \ 2\,\|f'\|_{L^2} \qquad \forall f \in C_0^\infty(\mathbb{R}^+)$$

implies

$$\|r^{-\frac{1}{2}}f\|_{L^2}^2 \ \leqslant \ \frac{\varepsilon}{4}\,\|r^{-1}f\|_{L^2}^2 + \frac{1}{\varepsilon}\,\|f\|_{L^2}^2 \ \leqslant \ \varepsilon\|f'\|_{L^2}^2 + \varepsilon^{-1}\|f\|_{L^2}^2$$

for arbitrary $\varepsilon > 0$. This and (4.2.18) imply on the one hand $\|f\|_F \lesssim \|f\|_{H^1}$, and on the other hand

$$\|f\|_F^2 \ \geqslant \ (1 - |\nu|\varepsilon)\|f'\|_{L^2}^2 + (1 + \tfrac{\nu^2}{4\,\kappa^2} - |\nu|\varepsilon^{-1})\|f\|_{L^2}^2\,.$$

The r.h.s. above is equivalent to the H^1-norm provided that the coefficients of $\|f'\|_{L^2}^2$ and $\|f\|_{L^2}^2$ are strictly positive, which is the same as

$$\nu^2 \ < \ \frac{|\nu|}{\varepsilon} \ < \ 1 + \frac{\nu^2}{4\,\kappa^2}\,.$$

For given ν and κ, a choice of $\varepsilon > 0$ satisfying the inequalities above is always possible, because $\nu^2 < 1 + \frac{\nu^2}{4\,\kappa^2}$, or equivalently, $1 + \nu^2(\frac{1}{4\kappa^2} - 1) > 0$, which is true owing to the assumption $0 < |\kappa| < \frac{1}{2}$. We have therefore shown that $\|f\|_F \approx \|f\|_{H^1}$ in the sense of the equivalence of norms on $C_0^\infty(\mathbb{R}^+)$. Now, the $\|\cdot\|_F$-completion of $C_0^\infty(\mathbb{R}^+)$ is by definition $\mathcal{D}[S_F]$, whereas the $\|\cdot\|_{H^1}$-completion is $H_0^1(\mathbb{R}^+)$: the Lemma is therefore proved. $\qquad\square$

Let us now highlight the following feature of $\operatorname{ran} R_G$.

Lemma 4.2.6. *For every $g \in L^2(\mathbb{R}^+)$ one has*

$$\int_0^{+\infty} \frac{|(R_G g)(r)|^2}{r^2} \mathrm{d}r \; < \; +\infty \,, \tag{4.2.20}$$

i.e.,

$$\operatorname{ran} R_G \subset \mathcal{D}(r^{-1}) \,. \tag{4.2.21}$$

Proof. It suffices to prove the finiteness of the integral in (4.2.20) only for $r \in (0,1)$, since $\int_1^{+\infty} r^{-2}|(R_G g)(r)|^2 \, \mathrm{d}r \leqslant \|R_G\|^2 \|g\|_{L^2}^2$. Owing to (4.2.14) and (4.2.16),

$$|(R_G g)(r)| \; \lesssim \; |\Phi_\kappa(r)| \int_0^r |F_\kappa(\rho)g(\rho)| \, \mathrm{d}\rho + |F_\kappa(r)| \int_0^{+\infty} |\Phi_\kappa(\rho)g(\rho)| \, \mathrm{d}\rho \,. \tag{*}$$

We then exploit the asymptotics (4.2.8). The first summand in the r.h.s. above as a $O(r^{3/2})$-quantity as $r \downarrow 0$, because in this limit Φ_κ is smooth and bounded, whereas F_κ is smooth and vanishes as $O(r)$, and therefore

$$\int_0^r |F_\kappa(\rho)g(\rho)| \, \mathrm{d}\rho \; \leqslant \; \sup_{\rho \in [0,r]} |F_\kappa(\rho)| \, \|g\|_{L^2} \, r^{1/2} \; = \; O(r^{3/2}) \,.$$

The second summand in the r.h.s. of (*) is a $O(r)$-quantity as $r \downarrow 0$, because so is $F_\kappa(r)$ and because $\int_0^{+\infty} |\Phi_\kappa(\rho)g(\rho)| \, \mathrm{d}\rho \leqslant \|\Phi_\kappa\|_{L^2}\|g\|_{L^2}$. Thus, $(R_G g)(r) = O(r)$ as $r \downarrow 0$, whence the integrability of $r^{-2}|(R_G g)(r)|^2$ at zero. $\qquad \square$

We can finally prove that $R_G = S_F^{-1}$.

Proof of Proposition 4.2.2. $R_G = \mathscr{S}^{-1}$ for some $\mathscr{S} = \mathscr{S}^* \supset S$ (Lemma 4.2.3), and we want to conclude that $\mathscr{S} = S_F$. This follows if we show that $\mathcal{D}(\mathscr{S}) \subset \mathcal{D}[S_F]$, owing to the well-known property of S_F that distinguishes it from all other self-adjoint extensions of S.

Let us then pick a generic $f = R_G g \in \operatorname{ran} R_G = \mathcal{D}(\mathscr{S})$ for some $g \in L^2(\mathbb{R}^+)$ and show that $S_F[f] := S_F[f,f] < +\infty$, the form of S_F being given by Lemma 4.2.4. The fact that $\|f\|_{L^2}^2$ is finite is obvious, and the finiteness of $\|r^{-\frac{1}{2}}f\|_{L^2}^2$ follows by interpolation from Lemma 4.2.6. We are thus left with proving that $\|f'\|_{L^2}^2 < +\infty$, and the conclusion then follows from (4.2.19).

Now, $f \in \mathcal{D}(S^*)$ and therefore $-f'' + \frac{\nu}{r}f + \frac{\nu^2}{4\,\kappa^2}f = g \in L^2(\mathbb{R}^+)$: this, and the already mentioned square-integrability of f and $r^{-1}f$, yield $f'' \in L^2(\mathbb{R}^+)$. It is then standard (see, e.g., [60, Remark 4.21]) to deduce that f' too belongs to $L^2(\mathbb{R}^+)$, thus concluding the proof. $\qquad \square$

For later purposes we set for convenience

$$\Psi_\kappa \; := \; S_F^{-1}\Phi_\kappa \; = \; R_G\Phi_\kappa \tag{4.2.22}$$

and we prove the following.

Lemma 4.2.7. *One has*

$$\Psi_\kappa(r) \; = \; \Gamma(1-\kappa)\|\Phi_\kappa\|_{L^2}^2 \, r + O(r^2) \qquad \text{as } r \downarrow 0 \,. \tag{4.2.23}$$

Proof. Owing to (4.2.14) and (4.2.16),

$$(R_G\Phi_\kappa)(r) \; = \; -\frac{\kappa\,\Gamma(1-\kappa)}{\nu}\left(\Phi_\kappa(r)\int_0^r F_\kappa(\rho)\Phi_\kappa(\rho)\,\mathrm{d}\rho + F_\kappa(r)\int_r^{+\infty}\Phi_\kappa^2(\rho)\,\mathrm{d}\rho\right).$$

As $r \downarrow 0$, (4.2.8) and (4.2.10) imply that the first summand behaves as

$$-\tfrac{\kappa\Gamma(1-\kappa)}{\nu}\left(\tfrac{1}{\Gamma(1-\kappa)}+O(r\ln r)\right)\int_0^r\left(-\tfrac{\nu}{\kappa}\rho+O(\rho^2)\right)\left(\tfrac{1}{\Gamma(1-\kappa)}+O(\rho\ln\rho)\right)\mathrm{d}\rho\,,$$

which, after some simplifications, becomes

$$\frac{1}{2\,\Gamma(1-\kappa)}\,r^2+O(r^3\ln r)\,.$$

The second summand turns out to be the leading term: indeed, as $r \downarrow 0$, $\int_r^\infty\Phi_\kappa^2\,\mathrm{d}\rho=\|\Phi_\kappa\|_{L^2(\mathbb{R}^+)}^2+O(r)$ and hence

$$-\frac{\kappa\,\Gamma(1-\kappa)}{\nu}\,F_\kappa(r)\int_r^{+\infty}\Phi_\kappa^2(\rho)\,\mathrm{d}\rho\;=\;\Gamma(1-\kappa)\|\Phi_\kappa\|_{L^2}^2\,r+O(r^2)\,,$$

which completes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\Box$

4.2.4   Operators $\overline{S}$, S_F, and S^*

In general (see Theorem 2.1.2 and (2.1.6)), the space $\mathcal{D}(S^*)$ implicitly qualified in (4.2.4) and the space $\mathcal{D}(S_F)$ have the following internal structure:

$$\begin{aligned}
\mathcal{D}(S^*) &= \mathcal{D}(\overline{S})\dotplus S_F^{-1}\ker S^*\dotplus\ker S^* &\qquad(4.2.24)\\
\mathcal{D}(S_F) &= \mathcal{D}(\overline{S})\dotplus S_F^{-1}\ker S^*\,. &\qquad(4.2.25)
\end{aligned}$$

Owing to (4.2.11) and to (4.2.22), this reads

$$\begin{aligned}
\mathcal{D}(S^*) &= \left\{g=f+c_1\Psi_\kappa+c_0\Phi_\kappa\,|\,f\in\mathcal{D}(\overline{S}),\,c_0,c_1\in\mathbb{C}\right\} &\qquad(4.2.26)\\
\mathcal{D}(S_F) &= \mathcal{D}(\overline{S})\dotplus\mathrm{span}\{\Psi_\kappa\}\,. &\qquad(4.2.27)
\end{aligned}$$

Let us focus on the space $\mathcal{D}(\overline{S})$. As observed, e.g., in [36, Prop. 3.1(i)-(ii)], the functions in $\mathcal{D}(\overline{S})$ display the following features.

Lemma 4.2.8. *Let $f\in\mathcal{D}(\overline{S})$. Then the functions f and f'*

(i) *are continuous on $\mathbb{R}^+$ and vanish as $r\to+\infty$;*

(ii) *vanish as $r\downarrow 0$ as*

$$f(r)=o(r^{3/2})\,,\qquad f'(r)=o(r^{1/2})\,. \qquad\qquad(4.2.28)$$

We can then conclude the following.

Lemma 4.2.9. *One has*

$$\mathcal{D}(\overline{S})\;=\;H_0^2(\mathbb{R}^+)\;=\;\overline{C_0^\infty(\mathbb{R}^+)}^{\|\,\|_{H^2}}\,. \qquad\qquad(4.2.29)$$

Proof. First we observe that

$$\mathcal{D}(\overline{S})\;\subset\;H_0^2(\mathbb{R}^+)\,. \qquad\qquad\qquad(\mathrm{i})$$

Indeed, for any $f\in\mathcal{D}(\overline{S})$ one has $\widetilde{S}f=-f''+\tfrac{\nu}{r}f+\tfrac{\nu^2}{4\kappa^2}f\in L^2(\mathbb{R}^+)$, as well as $f\in L^2(\mathbb{R}^+)$ and $r^{-1}f\in L^2(\mathbb{R}^+)$, the latter following from (4.2.28); therefore, $f''\in L^2(\mathbb{R}^+)$ and hence, as recalled already, necessarily $f\in H^2(\mathbb{R}^+)$. Owing to (4.2.28) again, $f(0)=f'(0)=0$, whence $f\in H_0^2(\mathbb{R}^+)$.

We also have the inclusion

$$H_0^2(\mathbb{R}^+)\;\subset\;\mathcal{D}(S^*)\,. \qquad\qquad\qquad(\mathrm{ii})$$

Indeed, for any $f \in H_0^2(\mathbb{R}^+)$ one has $f, f'' \in L^2(\mathbb{R}^+)$, and $f \in C_0^1(\mathbb{R}^+)$ by Sobolev's Lemma, where $C_0^1(\mathbb{R}^+)$ is the space of the C^1-functions over $\mathbb{R}^+$ vanishing at zero together with their derivative. Thus, $f(r) = o(r)$ as $r \downarrow 0$, implying $r^{-1}f \in L^2(\mathbb{R}^+)$. Then $\widetilde{S}f = -f'' + \frac{\nu}{r}f + \frac{\nu^2}{4\kappa^2}f \in L^2(\mathbb{R}^+)$, which by (4.2.4) means that $f \in \mathcal{D}(S^*)$.

We have then the chain

$$\begin{aligned} \mathcal{D}(\overline{S}) \;\subset\; H_0^2(\mathbb{R}^+) \;&\subset\; \mathcal{D}(S^*) \;=\; \mathcal{D}(\overline{S}) \dotplus \operatorname{span}\{\Psi_\kappa, \Phi_\kappa\} \\ &\subset\; H_0^2(\mathbb{R}^+) \dotplus \operatorname{span}\{\Psi_\kappa, \Phi_\kappa\} \;\subset\; \mathcal{D}(S^*)\,, \end{aligned}$$

where the first two inclusions are (i) and (ii) respectively, the identity that follows is an application of (4.2.26), then the next inclusion follows from (i) again and the sum remains direct because no non-zero element in $\operatorname{span}\{\Psi_\kappa, \Phi_\kappa\}$ belongs to $H_0^2(\mathbb{R}^+)$, and the last inclusion follows from (ii) and (4.2.26). Therefore,

$$\mathcal{D}(\overline{S}) \dotplus \operatorname{span}\{\Psi_\kappa, \Phi_\kappa\} \;=\; H_0^2(\mathbb{R}^+) \dotplus \operatorname{span}\{\Psi_\kappa, \Phi_\kappa\}\,, \quad \text{with } \mathcal{D}(\overline{S}) \subset H_0^2(\mathbb{R}^+)\,,$$

whence necessarily $\mathcal{D}(\overline{S}) = H_0^2(\mathbb{R}^+)$. $\qquad\square$

As a consequence, (4.2.27) now reads

$$\mathcal{D}(S_F) \;=\; H_0^2(\mathbb{R}^+) \dotplus \operatorname{span}\{\Psi_\kappa\} \tag{4.2.30}$$

and in addition we can qualify $\mathcal{D}(S_F)$ as follows.

Lemma 4.2.10. *One has*

$$\begin{aligned} \mathcal{D}(S_F) \;&=\; H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+) \\ &=\; \left\{ f \in H^2(\mathbb{R}^+) \,|\, f(0) = O(r) \text{ as } r \downarrow 0 \right\}. \end{aligned} \tag{4.2.31}$$

Proof. Based on (4.2.27) and (4.2.29), let $\phi = f + c\,\Phi_k \in \mathcal{D}(S_F)$ for generic $f \in H_0^2(\mathbb{R}^+)$ and $c \in \mathbb{C}$. From $-\Psi_\kappa'' + \frac{\nu}{r}\Psi_k + \frac{\nu^2}{4\kappa^2}\Psi_\kappa = S_F\Psi_\kappa = \Phi_\kappa \in L^2(\mathbb{R}^+)$ and from Lemma 4.2.6 one deduces that $\Psi_\kappa'' \in L^2(\mathbb{R}^+)$ and hence $\Psi_\kappa \in H^2(\mathbb{R}^+)$, which proves that $\mathcal{D}(S_F) \subset H^2(\mathbb{R}^+)$. Moreover, $\mathcal{D}(S_F) \subset \mathcal{D}[S_F] = H_0^1(\mathbb{R}^+)$, owing to Lemma 4.2.5, whence the conclusion $\mathcal{D}(S_F) \subset H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+)$.

For the converse inclusion, any $\phi \in H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+)$ is re-written as $\phi = f + \frac{\phi'(0)}{\Psi_\kappa'(0)}\Psi_\kappa$ with $f := \phi - \frac{\phi'(0)}{\Psi_\kappa'(0)}\Psi_\kappa$ (it is clear from the proof of Lemma 4.2.7 that $\Psi_\kappa'(0) = -\Gamma(1-\kappa)\|\Phi_\kappa\|_{L^2}^2 \neq 0$). By linearity $f \in H^2(\mathbb{R}^+)$, by the assumptions on ϕ and (4.2.23) $f(0) = 0$, and by construction $f'(0) = 0$. Thus, $f \in H_0^2(\mathbb{R}^+)$. Then $\phi \in \mathcal{D}(S_F)$ owing to (4.2.30). $\qquad\square$

In turn, we can now re-write (4.2.26) as

$$\begin{aligned} \mathcal{D}(S^*) \;&=\; H_0^2(\mathbb{R}^+) \dotplus \operatorname{span}\{\Psi_\kappa, \Phi_\kappa\} \\ &=\; \left(H^2(\mathbb{R}^+) \cap H_0^1(\mathbb{R}^+)\right) \dotplus \operatorname{span}\{\Phi_\kappa\}\,. \end{aligned} \tag{4.2.32}$$

To conclude this subsection we prove Theorem 4.1.1.

Proof of Theorem 4.1.1. Since $S - h_0^{(\nu)}$ is bounded, both $h_0^{(\nu)}$ and S have deficiency index one. Parts (i) and (ii) follow at once, respectively from Lemma 4.2.10 and Lemma 4.2.5, since the shift does not modify the domains. Concerning part (iii), it follows from

$$\left(h_{0,F}^{-1} + \frac{\nu^2}{4\kappa^2}\right)^{-1} \;=\; S_F^{-1} \;=\; R_G$$

and from the expression (4.2.16) for the kernel of R_G, using the definitions (4.2.10) and (4.2.14). $\quad\square$

4.2.5   Kreĭn-Višik-Birman classification of the extensions

Based on the Kreĭn-Višik-Birman extension theory presented in Chapter 2, applied to the present case of deficiency index one, the self-adjoint extensions of S correspond to those restrictions of S^* to subspaces of $\mathcal{D}(S^*)$ that, in terms of formula (4.2.26), are identified by the condition

$$c_1 \;=\; \beta c_0 \qquad \text{for some } \beta \in \mathbb{R} \cup \{\infty\} , \tag{4.2.33}$$

the extension parametrised by $\beta = \infty$ having the domain (4.2.30) and being therefore the Friedrichs extension.

Remark 4.2.11. If one replaces the restriction condition (4.2.33) with the same expression where now β is allowed to be a generic complex number, this gives all possible *closed* extensions of S between $\overline{S}$ and S^*, as follows by a straightforward application of Grubb's extension theory (see, e.g., [60, Chapter 13]), namely the natural generalisation of the Kreĭn-Višik-Birman theory for closed extensions. A recent application of Grubb's theory to operators of point interactions, including $(-\Delta)|_{C_0^\infty(\mathbb{R}^3 \setminus \{0\})}$ in $L^2(\mathbb{R}^3)$, from the point of view of Friedrichs systems, is presented in [39].

Let us denote with S_β the extension selected by (4.2.33) for given β. Owing to (4.2.26) and (4.2.33), a generic $g \in \mathcal{D}(S_\beta)$ decomposes as

$$g \;=\; f + \beta c_0 \Psi_\kappa + c_0 \Phi_\kappa \tag{4.2.34}$$

for unique $f \in H_0^2(\mathbb{R}^+)$ and $c_0 \in \mathbb{C}$. The asymptotics (4.2.8), (4.2.23), and (4.2.28) imply

$$
\begin{aligned}
g(r) \;=\;& \frac{c_0}{\Gamma(1-\kappa)} + \frac{c_0\,\nu}{\Gamma(1-\kappa)}\, r \ln r \\
&+ \left(c_0\, \nu\, \frac{2\psi(1-\kappa) + 2\ln(-\frac{\nu}{\kappa}) + (4\gamma - 2) + \kappa^{-1}}{2\,\Gamma(1-\kappa)} + c_0\, \beta\, \Gamma(1-\kappa) \|\Phi_\kappa\|^2 \right) r \\
&+ o(r^{3/2}) \qquad \text{as } r \downarrow 0 .
\end{aligned}
\tag{4.2.35}
$$

The $O(1)$-term and $O(r \ln r)$-term in (4.2.35) come from Φ_κ, and so does the first $O(r)$-term; the second $O(r)$-term comes instead from Ψ_κ; the $o(r^{3/2})$-remainder comes from f.

The analogous asymptotics for a generic function $g \in \mathcal{D}(S^*)$ is

$$g(r) \;=\; C_0 \Big(\frac{1}{\Gamma(1-\kappa)} + \frac{\nu}{\Gamma(1-\kappa)} r \ln r \Big) + C_1 r + o(r^{3/2}) \qquad \text{as } r \downarrow 0 \tag{4.2.36}$$

for some $C_0, C_1 \in \mathbb{C}$, as follows again from (4.2.8), (4.2.23), and (4.2.28) applied to (4.2.26). Comparing (4.2.35) with (4.2.36) we conclude the following.

Proposition 4.2.12 (Classification of extensions at $\ell = 0$: shift-dependent formulation)**.** *The self-adjoint extensions of S form a family $\{S_\beta \,|\, \beta \in \mathbb{R} \cup \{\infty\}\}$. The extension with $\beta = \infty$ is the Friedrichs extension S_F. For $\beta \in \mathbb{R}$, the extension S_β is the restriction of S^* to the domain $\mathcal{D}(S_\beta)$ that consists of all functions in $\mathcal{D}(S^*)$ for which the coefficient C_0 of the leading term $\frac{1}{\Gamma(1-\kappa)} + \frac{\nu}{\Gamma(1-\kappa)} r \ln r$ and the coefficient C_1 of the next $O(r)$-subleading term, as $r \downarrow 0$, are constrained by the relation*

$$\frac{C_1}{C_0} \;=\; c_{\nu,\kappa}\, \beta + d_{\nu,\kappa} , \tag{4.2.37}$$

where

$$
\begin{aligned}
c_{\nu,\kappa} \;&:=\; \Gamma(1-\kappa)\, \|\Phi_\kappa\|_{L^2}^2 \\
d_{\nu,\kappa} \;&:=\; \nu\, \frac{2\psi(1-\kappa) + 2\ln(-\frac{\nu}{\kappa}) + 2(2\gamma - 1) + \kappa^{-1}}{2\,\Gamma(1-\kappa)} .
\end{aligned}
\tag{4.2.38}
$$

Equivalently,

$$
\begin{aligned}
S_\beta &= S^* \upharpoonright \mathcal{D}(S_\beta) \\
\mathcal{D}(S_\beta) &= \left\{ g = f + \beta c_0 \Psi_\kappa + c_0 \Phi_\kappa \,\middle|\, f \in H_0^2(\mathbb{R}^+),\, c_0 \in \mathbb{C} \right\}.
\end{aligned}
\tag{4.2.39}
$$

Within the Kreĭn-Višik-Birman extension scheme an equivalent classification in terms of quadratic forms is available. In the present setting, Theorem 2.2.3 yields at once the following.

Proposition 4.2.13 (Shift-dependent classification at $\ell = 0$: form version)**.** *The self-adjoint extensions of S form a family $\{S_\beta \,|\, \beta \in \mathbb{R} \cup \{\infty\}\}$. The extension with $\beta = \infty$ is the Friedrichs extension S_F. For $\beta \in \mathbb{R}$, the extension S_β has quadratic form*

$$
\begin{aligned}
\mathcal{D}[S_\beta] &= \mathcal{D}[S_F] \dotplus \operatorname{span}\{\Phi_\kappa\} \\
S_\beta[\phi_\kappa + c_\kappa \Phi_\kappa] &= S_F[\phi_\kappa] + \beta|c_\kappa|^2 \|\Phi_\kappa\|_{L^2}^2
\end{aligned}
\tag{4.2.40}
$$

for generic $\phi_\kappa \in \mathcal{D}[S_F]$ and $c_\kappa \in \mathbb{C}$.

Thus, the classification provided by Proposition 4.2.12 identifies each extension *directly from the short distance behaviour of the elements of its domain*, and the self-adjointness condition (4.2.37) is a constrained *boundary condition* as $r \downarrow 0$ (see Remark 4.2.17 below for further comments). This turns out to be particularly informative for practical purposes, including our next purposes of classification of the discrete spectra of the S_β's.

The Friedrichs extension, $\beta = \infty$, is read out from (4.2.37) as $C_0 = 0$ and $C_1 = c_{\nu,k}$, upon interpreting $C_0\beta = 1$. In this case, as expected, (4.2.39) takes the form of (4.2.30) and (4.2.40) is interpreted as $\mathcal{D}[S_{\beta=\infty}] = \mathcal{D}[S_F]$. Moreover, the following feature of S_F is now obvious from (4.2.39) and from the short-distance asymptotics of Φ_κ and Ψ_κ given by (4.2.8) and (4.2.23) above.

Corollary 4.2.14. *The Friedrichs extension S_F is the* only *member of the family $\{S_\beta \,|\, \beta \in \mathbb{R} \cup \{\infty\}\}$ with operator domain contained in $\mathcal{D}[r^{-1}]$, i.e., it is the only self-adjoint extension whose domain's functions have finite expectation of the potential (and hence also of the kinetic) energy.*

Another immediate consequence of the extension parametrisation (4.2.39), as an application of Kreĭn's resolvent formula for deficiency index one 2.4.1, is the following.

Corollary 4.2.15. *The self-adjoint extension S_β is invertible if and only if $\beta \neq 0$, in which case*

$$
S_\beta^{-1} = S_F^{-1} + \frac{1}{\beta} \frac{1}{\|\Phi_\kappa\|^2} |\Phi_\kappa\rangle\langle\Phi_\kappa|.
\tag{4.2.41}
$$

Remark 4.2.16. Unlike the Friedrichs extension, the 'energy' $S_\beta[g]$ of an element $g \in \mathcal{D}[S_\beta]$ when $\beta \neq \infty$ differs from the formal expression $\|g'\|_{L^2}^2 + \nu\|r^{-\frac{1}{2}}g|\|\|_{L^2}^2 + \eta\|g\|_{L^2}^2$, $\eta = \frac{\nu^2}{4\kappa^2}$. The latter would be instead *infinite* for a generic g, and the *finiteness* of $S_\beta[g]$ can be interpreted as the effect of an infinite β-dependent correction to the above-mentioned formal expression such that the two infinities cancel out. Explicitly, let us write $g = \phi_\kappa + c_\kappa \Phi_\kappa$ as in (4.2.40) and compute

$$
\begin{aligned}
S_\beta[g] &= \|\phi_\kappa'\|_{L^2}^2 + \nu\|r^{-\frac{1}{2}}\phi_\kappa|\|\|_{L^2}^2 + \eta\|\phi_\kappa\|_{L^2}^2 + \beta|c_\kappa|^2 \|\Phi_\kappa\|_{L^2}^2 \\
&= \|g' - c_\kappa \Phi_\kappa'\|_{L^2}^2 + \nu\|r^{-\frac{1}{2}}(g - c_\kappa \Phi_\kappa)|\|\|_{L^2}^2 + \eta\|g - c_\kappa \Phi_\kappa\|_{L^2}^2 + \beta|c_\kappa|^2 \|\Phi_\kappa\|_{L^2}^2.
\end{aligned}
$$

'Opening the squares' in the above norms clearly yields infinities, so we only proceed formally here, understanding the following expressions as the $\varepsilon \downarrow 0$ limit of integrations that are supported on

$(\varepsilon, +\infty)$. One would then have

$$
\begin{aligned}
S_\beta[g] \;=\; & \|g'\|_{L^2}^2 + \nu\|r^{-\frac{1}{2}}g\|\|_{L^2}^2 + \eta\|g\|_{L^2}^2 \\
& + |c_\kappa|^2\Big(-\overline{\Phi_\kappa(0)}\,\Phi'_\kappa(0) + \int_0^{+\infty}\overline{\Phi_\kappa}\big(-\Phi''_\kappa + \tfrac{\nu}{r}\Phi_\kappa + \eta\Phi_\kappa\big)\,\mathrm{d}r\Big) \\
& - 2\,\mathfrak{Re}\,c_\kappa\Big(-\overline{g(0)}\,\Phi'_\kappa(0) + \int_0^{+\infty}\overline{g}\big(-\Phi''_\kappa + \tfrac{\nu}{r}\Phi_\kappa + \eta\Phi_\kappa\big)\,\mathrm{d}r\Big) \\
& + \beta|c_\kappa|^2\|\Phi_\kappa\|_{L^2}^2\,.
\end{aligned}
$$

Using that $-\Phi''_\kappa + \tfrac{\nu}{r}\Phi_\kappa + \eta\Phi_\kappa = 0$, $c_\kappa = g(0)/\Phi_\kappa(0)$, and Φ_κ is real-valued, we find

$$
S_\beta[g] \;=\; \|g'\|_{L^2}^2 + \nu\|r^{-\frac{1}{2}}g\|\|_{L^2}^2 + \eta\|g\|_{L^2}^2 + |g(0)|^2\Big(\frac{\Phi'_\kappa(0)}{\Phi_\kappa(0)} + \beta\,\frac{\|\Phi_\kappa\|_{L^2}^2}{|\Phi_\kappa(0)|^2}\Big).
$$

The β-dependent correction is now evident from the above expression, that must be interpreted as a *compensation* between the infinite 'formal form of g' given by the first three summands, and the infinite correction given by the fourth summand – observe indeed that $\Phi'_\kappa(r)/\Phi_\kappa(r) = (\nu\ln r)(1 + o(1))$ as $r\downarrow 0$. Only for the Friedrichs extension this correction is absent and $S_F[g]$ is given by the usual formula.

Remark 4.2.17. As mentioned in Section 4.1, our boundary-condition-driven classification of the self-adjoint realisations of the differential operator $\widetilde{S}$ on the half-line has several precursors in the literature [98, 21]. In fact, the analysis of radial Schrödinger operators with Coulomb potentials, and more generally of the so-called 'Whittaker operators' $-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + (\frac{1}{4}-\mu^2)\frac{1}{r^2} - \frac{\kappa}{r}$ on half-line, is also quite active in the present days [54, 19, 35, 36]. The very 'spirit' of the structural formula (4.2.39) is to link, through the extension parameter β, the 'regular' (in this context: rapidly vanishing) behaviour at the origin of the component $f + \beta c_0\Psi_\kappa$ with the 'singular' (non-vanishing) behaviour of the component $c_0\Phi_\kappa$ of a generic $g \in \mathcal{D}(S_\beta)$, and the boundary condition of self-adjointness (4.2.37) is a convenient re-phrasing of that. Lifting the analysis to the three dimensional case makes this terminology more appropriate, as remarked after Theorem 4.1.3.

The β-parametrisation in Propositions 4.2.12 and 4.2.13 is shift-dependent and it is convenient now to re-scale β so as to re-parametrise the extensions in a shift-independent way. To this aim, for $g \in \mathcal{D}(S^*)$ we set

$$
\begin{aligned}
g_0 &:= \frac{C_0}{\Gamma(1-\kappa)} \;=\; \lim_{r\downarrow 0} g(r) \\
g_1 &:= C_1 \;=\; \lim_{r\downarrow 0} r^{-1}\big(g(r) - g_0(1+\nu r\ln r)\big)
\end{aligned}
\tag{4.2.42}
$$

so that (4.2.36) reads

$$
g \;=\; g_0(1 + \nu\, r\ln r) + g_1 r + o(r^{3/2}) \qquad \text{as } r\downarrow 0\,,
\tag{4.2.43}
$$

and we also define

$$
\alpha \;:=\; \frac{1}{4\pi}\,\Gamma(1-\kappa)\,(c_{\nu,\kappa}\,\beta + d_{\nu,\kappa})\,.
\tag{4.2.44}
$$

Then, as obvious from (4.2.37)-(4.2.38),

$$
\mathcal{D}(S_\beta) \;=\; \{g \in \mathcal{D}(S^*)\,|\, g_1 = 4\pi\alpha g_0\}\,.
\tag{4.2.45}
$$

Moreover, an easy computation applying (4.2.44) yields

$$
\frac{1}{\beta}\frac{1}{\|\Phi_\kappa\|^2} \;=\; \frac{\Gamma(1-\kappa)^2}{4\pi}\,\frac{1}{\alpha - \frac{\nu}{4\pi}\big(\psi(1-\kappa) + \ln(-\frac{\nu}{\kappa}) + (2\gamma-1) + \frac{1}{2\kappa}\big)}\,.
\tag{4.2.46}
$$

This brings directly to the proof of our main result for the radial problem.

Proof of Theorem 4.1.2. Removing the shift from S to $h_0^{(\nu)}$ does not alter the domain of the corresponding self-adjoint extensions or adjoints, and modifies trivially their action. Thus, part (i) follows from Proposition 4.2.12 and from formulas (4.2.42) and (4.2.45) for $\mathcal{D}(S_\beta)$, using the expression (4.2.4) for $\mathcal{D}(S^*)$, whereas part (ii) follows from Corollary 4.2.15 with $S_\beta^{-1} = \left(h_{0,\alpha}^{(\nu)} + \frac{\nu^2}{4\kappa^2}\right)^{-1}$ and $S_F^{-1} = \left(h_{0,F}^{(\nu)} + \frac{\nu^2}{4\kappa^2}\right)^{-1}$, together with the identity (4.2.46). So far we have worked with $0 < |\kappa| < \frac{1}{2}$: thanks to the uniqueness of the analytic continuation, this determines unambiguously the resolvent at any point in the resolvent set. We can then extend all our previous formulas to the whole regime $(-\infty, 0) \cup (0, 1)$ for which the expression $\Gamma(1 - \kappa)$ still makes sense. $\qquad\square$

4.2.6   Reconstruction of the 3D hydrogenoid extensions

Finally, let us re-phrase the previous conclusions in terms of self-adjoint realisations of the hydrogenoid-type operator

$$\mathring{H}^{(\nu)} \;=\; -\Delta + \frac{\nu}{|x|}\,, \qquad \mathcal{D}(\mathring{H}^{(\nu)}) \;=\; C_0^\infty(\mathbb{R}^3 \backslash \{0\}) \tag{4.2.47}$$

(see (4.1.9) above) on $L^2(\mathbb{R}^3)$. The self-adjoint extensions of the shifted operator $\mathring{H}^{(\nu)} + \eta \mathbb{1}$, $\eta := \frac{\nu^2}{4\kappa^2}$, in the sector of angular symmetry $\ell = 0$ of $L^2(\mathbb{R}^3)$ are precisely those found in Proposition 4.2.12.

Proof of Theorem 4.1.3.
   Part (i). Formula (4.1.22) is obvious from (4.1.11)-(4.1.12) and from Theorem 4.1.2.

   Part (ii). Obviously the unique self-adjoint extension of $\mathring{H}^{(\nu)}$, hence necessarily the Friedrichs extension, in the sectors with angular symmetry $\ell \geqslant 1$ is the projection onto such sectors of the operator (4.1.24), owing to part (i) of this theorem. In the sector $\ell = 0$ the operator (4.1.24) acts as $\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\nu}{r}\right) \otimes \mathbb{1}$ and it remains to recognise that its radial domain consists of those f's in $H^2(\mathbb{R}^+)$ that vanish as $f(r) = O(r)$ as $r \downarrow 0$, because this is precisely $\mathcal{D}(S_F)$. This is standard: spherically symmetric elements of $H^2(\mathbb{R}^3)$ are functions $F(|x|)$ for $F \in L^2(\mathbb{R}^+, r^2\,\mathrm{d}r)$ such that $\Delta_x F \in L^2(\mathbb{R}^3, \mathrm{d}x)$ and hence $\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\frac{\mathrm{d}}{\mathrm{d}r}F) \in L^2(\mathbb{R}^+, r^2\mathrm{d}r)$; on the other hand $F = \frac{f}{r}$ for $f \in L^2(\mathbb{R}^+, \mathrm{d}r)$, whence $\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\frac{\mathrm{d}}{\mathrm{d}r}F) = \frac{f''}{r}$, and the square-integrability of $\Delta_x F$ reads $f'' \in L^2(\mathbb{R}^+, \mathrm{d}r)$; therefore, $f \in H^2(\mathbb{R}^+)$ and $f(r) = rF(r) = O(r)$ as $r \downarrow 0$. Last, the feature mentioned in the statement which identifies uniquely the Friedrichs extension follow from Proposition 4.2.12 and Corollary 4.2.14, thanks to the equivalence $\alpha = \infty \Leftrightarrow \beta = \infty$.

   Part (iii). Owing to parts (i) and (ii) we only have to establish (4.1.25) over the sector $\ell = 0$. In this sector, *radially,*

$$\left(h_{0,\alpha}^{(\nu)} + \tfrac{\nu^2}{4\kappa^2}\mathbb{1}\right)^{-1} \;=\; \left(h_{0,\infty}^{(\nu)} + \tfrac{\nu^2}{4\kappa^2}\mathbb{1}\right)^{-1} + \frac{1}{\beta}\frac{1}{\|\Phi_\kappa\|^2}|\Phi_\kappa\rangle\langle\Phi_\kappa|$$

owing to Corollary 4.2.15. Formula (4.1.26) reads

$$\mathfrak{g}_{\nu,k}(x) \;=\; \frac{\Gamma(1-\kappa)}{4\pi}\frac{\Phi_\kappa(|x|)}{|x|} \;=\; \frac{\Gamma(1-\kappa)}{\sqrt{4\pi}}\frac{\Phi_\kappa(|x|)}{|x|} \otimes Y_0^0$$

and therefore the projection $|\mathfrak{g}_{\nu,k}\rangle\langle\mathfrak{g}_{\nu,k}|$ acting on $L^2(\mathbb{R}^3)$ acts radially in the $\ell = 0$ sector as the projection $\frac{\Gamma(1-\kappa)^2}{4\pi}|\Phi_\kappa\rangle\langle\Phi_\kappa|$. This proves that

$$\left(H_\alpha^{(\nu)} + \frac{\nu^2}{4\kappa^2}\mathbb{1}\right)^{-1} \;=\; \left(H^{(\nu)} + \frac{\nu^2}{4\kappa^2}\mathbb{1}\right)^{-1} + \frac{1}{\beta}\frac{1}{\|\Phi_\kappa\|^2}\frac{4\pi}{\Gamma(1-\kappa)^2}|\mathfrak{g}_{\nu,k}\rangle\langle\mathfrak{g}_{\nu,k}|\,.$$

Combining the formula above with (4.2.46) finally yields the resolvent formula (4.1.25).

   Part (iv). This is a standard consequence of part (ii) – see, e.g., the argument in the proof of [4, Theorems I.1.1.3 and I.2.1.2]. $\qquad\square$

4.3   Perturbations of the discrete spectra

In this Section we prove Theorem 4.1.4 and we add a few additional observations.

We deliberately choose another path as compared to the standard approach [126, 3, 21] that determines the eigenvalues as poles of the resolvent (4.1.25) (see Remark 4.3.5 below), and we exploit instead the radial analysis of extensions that we have developed in Sec. 4.2. This completes our approach based on the Kreĭn-Višik-Birman extension theory.

4.3.1   The s-wave eigenvalue problem

For fixed $\alpha \in \mathbb{R}$ and $\nu \in \mathbb{R}$ let $\Psi \in \mathcal{D}(H_\alpha^{(\nu)})$ and $E < 0$ satisfy $H_\alpha^{(\nu)}\Psi = E\Psi$ with Ψ belonging to the L^2-sector with angular symmetry $\ell = 0$.

In view of (4.1.11) we write

$$\Psi(x) \;=\; \frac{g(|x|)}{\sqrt{4\pi}\,|x|} \tag{4.3.1}$$

for some $g \in \mathcal{D}(S_\beta) \subset L^2(\mathbb{R}^+)$ such that $S_\beta g = (E + \frac{\nu^2}{4\kappa^2})g$, where β is given by (4.2.44) for the chosen α and ν, and a chosen $\kappa \in (0,1)$ (see (4.2.2) above). Thus,

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\nu}{r}\right)g \;=\; Eg\,. \tag{4.3.2}$$

Passing to re-scaled energy $\mathfrak{e}$, radial variable ρ, coupling ϑ, and unknown h defined by

$$\begin{aligned}
\mathfrak{e} &:= \frac{4\kappa^2 E}{\nu^2} + 1\,, & \rho &:= -r\,\frac{\nu\sqrt{1-\mathfrak{e}}}{\kappa} \;=\; 2r\sqrt{|E|} \\
\vartheta &:= \frac{\kappa}{\sqrt{1-\mathfrak{e}}} \;=\; \frac{-\nu}{2\sqrt{|E|}}\,, & u(\rho) &:= g(r)\,,
\end{aligned} \tag{4.3.3}$$

the eigenvalue problem (4.3.2) takes the form

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{\vartheta}{\rho} + \frac{1}{4}\right)u \;=\; 0\,, \tag{4.3.4}$$

namely a Whittaker equation of the same type (4.2.5) above, whose only square-integrable solutions on $\mathbb{R}^+$, analogously to what argued in Section 4.2.1, are the multiples of Whittaker's function

$$u(\rho) \;=\; \mathscr{W}_{\vartheta,\frac{1}{2}}(\rho) \;=\; e^{-\frac{1}{2}\rho}\,\rho\, U_{1-\vartheta,2}(\rho)\,. \tag{4.3.5}$$

Therefore, up to multiples, the solution to (4.3.2) is

$$g(r) \;=\; \mathscr{W}_{\vartheta,\frac{1}{2}}\big(2r\sqrt{|E|}\big)\,. \tag{4.3.6}$$

By means of the expansion (4.2.8) and of the identity $\nu = -2\sqrt{|E|}\,\vartheta$ one finds

$$\begin{aligned}
g_0 &= \frac{1}{\Gamma\big(1 + \frac{\nu}{2\sqrt{|E|}}\big)} \\
g_1 &= \nu\,\frac{\psi\big(1 + \frac{\nu}{2\sqrt{|E|}}\big) + \ln(2\sqrt{|E|}) + 2\gamma - 1 - \frac{\sqrt{|E|}}{\nu}}{\Gamma\big(1 + \frac{\nu}{2\sqrt{|E|}}\big)}\,,
\end{aligned} \tag{4.3.7}$$

and such two constants must satisfy the condition $g_1 = 4\pi\alpha g_0$, as prescribed by Theorem 4.1.2 , because the considered eigenfunction Ψ belongs to $\mathcal{D}(H_\alpha^{(\nu)})$. We have thus proved that E is an eigenvalue for $H_\alpha^{(\nu)}$ if and only if

$$\mathfrak{F}_\nu(E) \;=\; \alpha \tag{4.3.8}$$
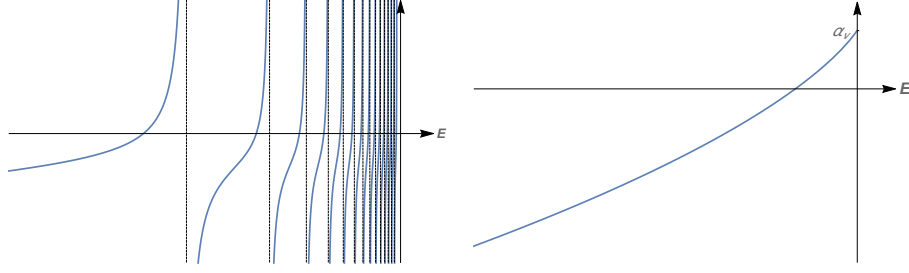
Figure 4.2: Behaviour of the function $(-\infty, 0) \ni E \mapsto \mathfrak{F}_\nu(E)$ for $\nu < 0$ (left) and $\nu > 0$ (right). Dashed lines in the figure represent vertical asymptotes.

with $\mathfrak{F}_\nu$ defined in (4.1.29).

When $\nu < 0$ the function $(-\infty, 0) \ni E \mapsto \mathfrak{F}_\nu(E)$ has vertical asymptotes corresponding to non-positive arguments $1 + \frac{\nu}{2\sqrt{|E|}} = -q$, $q \in \mathbb{N}_0$, of the digamma function ψ, i.e., at the points $E = E_n^{(\nu)}$ defined by

$$E_n^{(\nu)} \ := \ -\frac{\nu^2}{4n^2}\,, \qquad n := q + 1 \in \mathbb{N}. \tag{4.3.9}$$

The sequence $(E_n)_{n \in \mathbb{N}}$ is increasing and converges to zero. Within each interval (E_n, E_{n+1}) the function $E \mapsto \mathfrak{F}_\nu(E)$ is smooth and strictly monotone increasing, and moreover

$$\lim_{E \to -\infty} \mathfrak{F}_\nu(E) \ = \ -\infty\,.$$

Thus, for any $\alpha \in \mathbb{R}$ does the equation (4.3.8) admit countably many negative simple roots, which form the increasing sequence $(E_n^{(\nu,\alpha)})_{n \in \mathbb{N}}$ and accumulate at zero. Therefore, the s-wave point spectrum of $H_\alpha^{(\nu)}$ consists precisely of the $E_n^{(\nu,\alpha)}$'s. In the extremal case $\alpha = \infty$ one has $E_n^{(\nu,\alpha=\infty)} = E_n^{(\nu)}$: indeed, the s-wave point spectrum of the Friedrichs extension $H^{(\nu)}$ is the ordinary non-relativistic hydrogenoid s-wave spectrum, as given by (4.3.9).

When $\nu > 0$ the function $(-\infty, 0) \ni E \mapsto \mathfrak{F}_\nu(E)$ is smooth and strictly monotone increasing, with

$$\lim_{E \to -\infty} \mathfrak{F}_\nu(E) = -\infty\,, \qquad \lim_{E \uparrow 0} \mathfrak{F}_\nu(E) \ = \ \frac{\nu}{4\pi}\,(\ln \nu + 2\gamma - 1) \ =: \ \alpha_\nu\,,$$

the latter limit following from (4.1.29) owing to the asymptotics [1, Eq. (6.3.18)] that here reads

$$\psi\Big(1 + \frac{\nu}{2\sqrt{|E|}}\Big) \ \overset{E \to 0}{=} \ \ln \frac{\nu}{2\sqrt{|E|}} + O(\sqrt{|E|})\,.$$

Thus, the equation (4.3.8) has no negative roots if $\alpha \geqslant \alpha_\nu$ and one negative root if $\alpha < \alpha_\nu$.

This completes the proof of Theorem 4.1.4.

4.3.2 Further remarks

Remark 4.3.1. The result of Theorem 4.1.4 when $\nu < 0$ confirms that $H^{(\nu)} \geqslant H_\alpha^{(\nu)}$, namely that the Friedrichs extension is larger (in the sense of self-adjoint operator ordering) than any other extension. In particular, $E_{n+1}^{(\nu,\alpha)} \geqslant E_n^{(\nu)} \geqslant E_n^{(\nu,\alpha)}$.

Remark 4.3.2. As is clear from the behaviour of the roots to $\mathfrak{F}_\nu(E) = \alpha$ (Fig. 4.2)

$$\bigcup_\alpha \sigma_{\mathrm{p}}^{(0)}(H_\alpha^{(\nu)}) \ = \ (-\infty, 0)\,. \tag{4.3.10}$$

In this sense the spectra $\sigma_{\mathrm{p}}^{(0)}(H_\alpha^{(\nu)})$ fibre, as α runs over $\mathbb{R} \cup \{\infty\}$, the whole negative real line.

Remark 4.3.3. When $\nu < 0$ one has

$$\lim_{\alpha \to -\infty} E_1^{(\nu,\alpha)} \;=\; -\infty\,, \qquad \lim_{\alpha \to -\infty} E_{n+1}^{(\nu,\alpha)} \;=\; E_n^{(\nu)}\,, \quad n = 2, 3, \ldots$$

Both limits are obvious from the behaviour of the function $\mathfrak{F}_\nu(E)$ (Fig. 4.2); the former in particular is a consequence of general facts of the Kreĭn-Višik-Birman theory, in the following sense. That there exists only one eigenvalue of $H_\alpha^{(\nu)}$ below the bottom $E_1^{(\nu)}$ of the Friedrichs extension $H^{(\nu)}$ is a consequence of $\mathring{H}^{(\nu)}$ having deficiency index one and of the general result (see Corollary 2.3.10). Moreover, such eigenvalue, which is precisely $E_1^{(\nu,\alpha)}$, must satisfy

$$E_1^{(\nu,\alpha)} \;\leqslant\; \beta \;=\; \frac{1}{c_{\nu,\kappa}}\Big(\frac{4\pi\alpha}{\Gamma(1-\kappa)} - d_{\nu,\kappa}\Big)$$

for any fixed $\kappa \in (0,1)$, as a consequence of (4.2.44) and of the general property of Theorem 2.3.9. Thus, the limit $\alpha \to -\infty$ in the above inequality reproduces the limit for $E_1^{(\nu,\alpha)}$.

Remark 4.3.4. When $\nu > 0$ Theorem 4.1.4 implies that $H_\alpha^{(\nu)} \geqslant \mathbb{O}$ if and only if $\alpha \geqslant \alpha_\nu$. This fact too can be understood in terms of a general property of the Kreĭn-Višik-Birman theory [51, Theorem 3.5], which in the present setting reads

$$H_\alpha^{(\nu)} + \frac{\nu^2}{4\kappa^2}\mathbb{1} \;\geqslant\; \mathbb{O} \qquad \Leftrightarrow \qquad \beta \geqslant 0$$

for any $\kappa < 0$. The limit $\kappa \to -\infty$ and (4.2.44) then yields

$$\begin{aligned}
H_\alpha^{(\nu)} \;\geqslant\; \mathbb{O} \qquad \Leftrightarrow \qquad \alpha \;&\geqslant\; \lim_{\kappa \to -\infty} \frac{\Gamma(1-\kappa)}{4\pi}\, d_{\nu,\kappa} \\
&= \; \lim_{\kappa \to -\infty} \frac{\nu}{4\pi}\left(\psi(1-\kappa) + \ln(-\tfrac{\nu}{\kappa}) + 2\gamma - 1 + \tfrac{1}{2\kappa}\right) \\
&= \; \frac{\nu}{4\pi}\left(\ln\nu + 2\gamma - 1\right) \;=\; \alpha_\nu\,,
\end{aligned}$$

the limit above following again from the asymptotics [1, Eq. (6.3.18)].

Remark 4.3.5. Having identified the eigenvalues of $H_\alpha^{(\nu)}$ as the roots of $\mathfrak{F}_\nu(E) = \alpha$ is clearly consistent with the fact that such eigenvalues are all the poles of the resolvent $(H_\alpha^{(\nu)} - z\mathbb{1})^{-1}$, $z = -\frac{\nu^2}{4\kappa^2}$, determined in (4.1.25), i.e., the values $E = -\frac{\nu^2}{4\kappa^2}$ with κ determined by $\mathfrak{F}_{\nu,\kappa} = \alpha$, which is precisely another way of writing $\mathfrak{F}_\nu(E) = \alpha$.

Chapter 5

Dirac-Coulomb Operators in the Critical Regime

5.1 Introduction and Main results

In quantum mechanics a relativistic electron or positron (or more generally a relativistic spin-$\frac{1}{2}$ particle) which moves freely in the three-dimensional space is described by elements of the Hilbert space

$$\mathcal{H} := L^2(\mathbb{R}^3) \otimes \mathbb{C}^4 \cong L^2(\mathbb{R}^3, \mathbb{C}^4, \mathrm{d}x) \tag{5.1.1}$$

and by the (formal) Hamiltonian

$$H_0 := -\mathrm{i}c\hbar\,\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta mc^2 \tag{5.1.2}$$

acting on $\mathcal{H}$, where $\hbar$ is Planck's constant, c is the speed of light, m is the mass of the particle, and $\boldsymbol{\alpha} \equiv (\alpha_1, \alpha_2, \alpha_3)$ and β are the 4×4 matrices

$$\beta = \begin{pmatrix} \mathbb{1} & \mathbb{O} \\ \mathbb{O} & -\mathbb{1} \end{pmatrix}, \qquad \alpha_j = \begin{pmatrix} \mathbb{O} & \sigma_j \\ \sigma_j & \mathbb{O} \end{pmatrix}, \qquad j \in \{1,2,3\}, \tag{5.1.3}$$

having denoted by $\mathbb{1}$ and $\mathbb{O}$, respectively, the identity and the zero 2×2 matrix, and by σ_j, as customary, the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.1.4}$$

Explicitly, the scalar product between any two elements $\psi \equiv (\psi_1, \psi_2, \psi_3, \psi_4)$ and $\phi \equiv (\phi_1, \phi_2, \phi_3, \phi_4)$ in $\mathcal{H}$ is given by

$$\langle \psi, \phi \rangle_{\mathcal{H}} = \sum_{j=1}^{4} \int_{\mathbb{R}^3} \overline{\psi_j(x)}\, \phi_j(x)\, \mathrm{d}x, \tag{5.1.5}$$

and H_0 is the first order matrix-valued differential operator

$$H_0 = \begin{pmatrix} mc^2\,\mathbb{1} & -\mathrm{i}\hbar c\,\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \\ -\mathrm{i}\hbar c\,\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} & -mc^2\,\mathbb{1} \end{pmatrix} \tag{5.1.6}$$

(where $\boldsymbol{\sigma} \equiv (\sigma_1, \sigma_2, \sigma_3)$), known as the free Dirac operator.

The properties of H_0 are well known [111]. H_0 is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3 \backslash \{0\}, \mathbb{C}^4)$ with domain of self-adjointness

$$H^1(\mathbb{R}^3) \otimes \mathbb{C}^4 \cong H^1(\mathbb{R}^3, \mathbb{C}^4), \tag{5.1.7}$$

and its spectrum (as a self-adjoint operator on $\mathcal{H}$) is purely absolutely continuous and given by

$$\sigma(H_0) \;=\; \sigma_{\mathrm{ac}}(H_0) \;=\; (-\infty, -mc^2] \cup [mc^2, +\infty)\,. \tag{5.1.8}$$

In fact, H_0 is unitarily equivalent to

$$\widetilde{H_0} \;:=\; \begin{pmatrix} \mathbb{1}\sqrt{-c^2\Delta + m^2 c^4} & 0 \\ 0 & -\mathbb{1}\sqrt{-c^2\Delta + m^2 c^4} \end{pmatrix}. \tag{5.1.9}$$

When the particle is subject to the external scalar field due to the Coulomb interaction with a nucleus of atomic number Z placed in the origin of $\mathbb{R}^3$, this is accounted for by the so-called Dirac-Coulomb Hamiltonian

$$H \;:=\; -\mathrm{i}c\hbar\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 - \frac{e^2 Z}{\hbar\,|x|}\mathbb{1} \;=\; H_0 - \frac{cZ\alpha_{\mathrm{f}}}{|x|}\mathbb{1}\,, \tag{5.1.10}$$

where now $\mathbb{1}$ is the 4×4 identity matrix (no confusion should arise here and henceforth on the symbol $\mathbb{1}$, being its meaning of identity self-explanatory from the context), e is the elementary charge, and

$$\alpha_{\mathrm{f}} \;=\; \frac{e^2}{\hbar c} \;\approx\; \frac{1}{137} \tag{5.1.11}$$

is the fine-structure constant. The operator H can at least be defined minimally on $C_0^\infty(\mathbb{R}^3\backslash\{0\}, \mathbb{C}^4)$, in which case it is densely defined and symmetric on $\mathcal{H}$. However, the possibility that this yields an unambiguous physical realisation of H depends on the magnitude of the coupling $Z\alpha_{\mathrm{f}}$, hence of the nuclear charge Z. It is indeed well known [111] that the formal operator (5.1.10) is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3\backslash\{0\}, \mathbb{C}^4)$ *only* when $Z\alpha_{\mathrm{f}} \leqslant \frac{\sqrt{3}}{2}$ (i.e., $Z \leqslant 118$), in which case the domain of self-adjointness is $\mathcal{D}(H) = \mathcal{D}(H_0) = H^1(\mathbb{R}^3, \mathbb{C}^4)$ and the spectrum consists of the same essential part $\sigma_{\mathrm{ess}}(H) = (-\infty, -mc^2] \cup [mc^2, +\infty)$ as for H_0, plus a discrete spectrum in the 'gap' $(-mc^2, mc^2)$ consisting of eigenvalues $E_{n,\kappa}$ given by Sommerfeld's celebrated fine-structure formula

$$E_{n,\kappa} \;=\; mc^2\Big(1 + \frac{(Z\alpha_{\mathrm{f}})^2}{\big(n + \sqrt{\kappa^2 - (Z\alpha_{\mathrm{f}})^2}\,\big)^2}\Big)^{-\frac{1}{2}}, \quad n \in \mathbb{N}_0,\, \kappa \in \mathbb{Z}\backslash\{0\}\,. \tag{5.1.12}$$

Although the above regime of Z covers all currently known elements (the last one to be discovered, the Oganesson $^{294}_{118}$Og, thus $Z = 118$, was first synthesized in 2002 and formally named in 2016), the problem of the self-adjoint realisation of the Dirac-Coulomb Hamiltonian above the threshold $Z\alpha_{\mathrm{f}} = \frac{\sqrt{3}}{2}$ has been topical since long and so is still today. Even the consideration that the problem only arises due to the idealisation of point-like nuclei (and also because one neglects the anomalous magnetic moment of the electron) does not diminish its relevance, given the extreme experimental precision, for example, of Sommerfeld's fine-structure formula for the eigenvalues of H when $Z \leqslant 118$.

From the mathematical side, the study of the self-adjoint extensions of the Dirac-Coulomb Hamiltonian has a long and active history [42, 117, 97, 103, 102, 61, 122, 68, 89, 123, 28, 72, 76, 78, 77, 22, 9, 8, 70, 13, 111, 124, 53, 41, 114, 10, 11, 64, 40, 26, 27]. For the clarity of presentation, let us adopt natural units $c = \hbar = m = e = 1$ henceforth, so as to get rid of mathematically inessential parameters, the coupling constant of relevance thus becoming $\nu \equiv -Z\alpha_{\mathrm{f}}$.

Theorem 5.1.1 (Self-adjoint extensions of the minimal Dirac-Coulomb)**.** *On the Hilbert space* $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4, \mathrm{d}x)$ *consider, for fixed* $\nu \in \mathbb{R}$, *the operator*

$$H \;=\; H_0 + \frac{\nu}{|x|}\mathbb{1}\,, \qquad H_0 \;=\; -\mathrm{i}\,\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta\,,$$
$$\mathcal{D}(H) \;=\; \mathcal{D}(H_0) \;=\; C_0^\infty(\mathbb{R}^3\backslash\{0\}, \mathbb{C}^4)\,. \tag{5.1.13}$$

H_0 *is essentially self-adjoint and the domain (of self-adjointness) of its operator closure* $\overline{H_0}$ *is* $H^1(\mathbb{R}^3, \mathbb{C}^4)$. *Moreover, the following holds.*

(i) (Sub-critical regime.) *If $|\nu| \leqslant \frac{\sqrt{3}}{2}$, then H is essentially self-adjoint and $\mathcal{D}(\overline{H}) = H^1(\mathbb{R}^3, \mathbb{C}^4)$.*

(ii) (Critical regime.) *If $\frac{\sqrt{3}}{2} < |\nu| < 1$, then H admits an infinity of self-adjoint extensions, among which there is a 'distinguished' one, H_D, uniquely characterised by the properties*

$$\mathcal{D}(H_D) \subset \mathcal{D}(|H_0|^{1/2}) \quad \text{or} \quad \mathcal{D}(H_D) \subset \mathcal{D}(|x|^{-1/2}), \tag{5.1.14}$$

that is, the unique extension whose operator domain is both in the kinetic energy form domain $\mathcal{D}[H_0] = \mathcal{D}(|H_0|^{1/2})$ and in the potential energy form domain $\mathcal{D}[|x|^{-1}] = \mathcal{D}(|x|^{-1/2})$. Moreover, $0 \notin \sigma(H_D)$.

(iii) (Super-critical regime.) *If $|\nu| \geqslant 1$, then H admits an infinity of self-adjoint extensions, without a distinguished one in the sense of the operator H_D in the critical regime. In fact, when $|\nu| > 1$ every self-adjoint extension of H has infinitely many eigenfunctions not belonging to $\mathcal{D}(|x|^{-1/2})$.*

In either regime, the spectrum of any self-adjoint extension $\widetilde{H}$ of H is such that

$$\begin{aligned} \sigma_{\mathrm{ess}}(\widetilde{H}) &= \sigma(\overline{H_0}) = (-\infty, -1] \cup [1, +\infty) \\ \sigma_{\mathrm{disc}}(\widetilde{H}) &\subset (-1, 1). \end{aligned} \tag{5.1.15}$$

It is worth remarking that for Coulomb-like matrix-valued interactions $V(x)$ that are *not* of the form $\nu|x|^{-1}\mathbb{1}$ but still satisfy $|V(x)| \leqslant \nu|x|^{-1}$, the sub-critical regime described in Theorem 5.1.1(i) only ranges up to $|\nu| < \frac{1}{2}$, and counterexamples are well known of operators $H_0 + V$ with $|V(x)| \leqslant (\frac{1}{2}+\varepsilon)|x|^{-1}$ for arbitrary $\varepsilon > 0$ and failing to be essentially self-adjoint on $C_0^\infty(\mathbb{R}^3\backslash\{0\}, \mathbb{C}^4)$ [8].

In this chapter we are primarily focused on the critical regime, $|\nu| \in (\frac{\sqrt{3}}{2}, 1)$. This is a regime of ultra-heavy nuclei, in fact nuclei of elements that one expects to discover in the next future. It is the first regime where the Kato-Rellich-like perturbative arguments, applicable for small ν's, cease to work. It is also regarded as a physically meaningful regime, because as long as $|\nu| < 1$ Sommerfeld's fine-structure formula still provides, formally, bound states for real energy levels, which only become complex when $|\nu| > 1$, thus predicting an instability of the atom (the '$Z = 137$ catastrophe').

In order to give a first formulation of our main result, let us exploit, as customary, the canonical decomposition of H into partial wave operators [111, Section 4.6], which is induced by its spherical symmetry. By expressing $x \equiv (x_1, x_2, x_3) \in \mathbb{R}^3$ in polar coordinates $x = (r, \Omega) \in \mathbb{R}^+ \times \mathbb{S}^2$, $r := |x|$, the map $\psi(x) \mapsto r\psi(x_1(r, \Omega), x_2(r, \Omega), x_3(r, \Omega))$ induces a unitary isomorphism

$$L^2(\mathbb{R}^3, \mathbb{C}^4, \mathrm{d}x) \xrightarrow{\cong} L^2(\mathbb{R}^+, \mathrm{d}r) \otimes L^2(\mathbb{S}^2, \mathbb{C}^4, \mathrm{d}\Omega).$$

In terms of the observables

$$\begin{aligned} \boldsymbol{L} &= \boldsymbol{x} \times (-\mathrm{i}\boldsymbol{\nabla}), & \boldsymbol{S} &= -\frac{1}{4}\boldsymbol{\alpha} \times \boldsymbol{\alpha}, \\ \boldsymbol{J} &= \boldsymbol{L} + \boldsymbol{S} \equiv (J_1, J_2, J_3), & K &= \beta(2\boldsymbol{L} \cdot \boldsymbol{S} + \mathbb{1}), \end{aligned}$$

one further decomposes

$$L^2(\mathbb{S}^2, \mathbb{C}^4, \mathrm{d}\Omega) \cong \bigoplus_{j \in \frac{1}{2}\mathbb{N}} \bigoplus_{m_j=-j}^{j} \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{K}_{m_j, \kappa_j}, \tag{5.1.16}$$

where

$$\mathcal{K}_{m_j, \kappa_j} := \mathrm{span}\{\Psi_{m_j, \kappa_j}^+, \Psi_{m_j, \kappa_j}^-\} \cong \mathbb{C}^2 \tag{5.1.17}$$

and $\Psi^+_{m_j,\kappa_j}$ and $\Psi^-_{m_j,\kappa_j}$ are two orthonormal vectors in $\mathbb{C}^4$, and simultaneous eigenvectors of the observables $J^2 \upharpoonright L^2(\mathbb{S}^2,\mathbb{C}^4,\mathrm{d}\Omega)$, $J_3 \upharpoonright L^2(\mathbb{S}^2,\mathbb{C}^4,\mathrm{d}\Omega)$, and $K \upharpoonright L^2(\mathbb{S}^2,\mathbb{C}^4,\mathrm{d}\Omega)$ with eigenvalue, respectively, $j(j+1)$, m_j, and κ_j. It then turns out that each subspace

$$\mathcal{H}_{m_j,\kappa_j} := L^2(\mathbb{R}^+,\mathrm{d}r) \otimes \mathcal{K}_{m_j,\kappa_j} \cong L^2(\mathbb{R}^+,\mathbb{C}^2,\mathrm{d}r) \tag{5.1.18}$$

is a reducing subspace for the Dirac-Coulomb Hamiltonian H, which, through the overall isomorphism

$$U \;:\; L^2(\mathbb{R}^3,\mathbb{C}^4,\mathrm{d}x) \;\xrightarrow{\;\cong\;}\; \bigoplus_{j\in\frac{1}{2}\mathbb{N}} \; \bigoplus_{m_j=-j}^{j} \; \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} \mathcal{H}_{m_j,\kappa_j}\,, \tag{5.1.19}$$

is therefore unitarily equivalent to

$$U H U^* \;=\; \bigoplus_{j\in\frac{1}{2}\mathbb{N}} \; \bigoplus_{m_j=-j}^{j} \; \bigoplus_{\kappa_j=\pm(j+\frac{1}{2})} h_{m_j,\kappa_j}\,, \tag{5.1.20}$$

where

$$h_{m_j,\kappa_j} := \begin{pmatrix} 1 + \frac{\nu}{r} & -\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa_j}{r} \\ \frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa_j}{r} & -1 + \frac{\nu}{r} \end{pmatrix}, \tag{5.1.21}$$

$$\mathcal{D}(h_{m_j,\kappa_j}) := C_0^\infty(\mathbb{R}^+) \otimes \mathcal{K}_{m_j,\kappa_j} \cong C_0^\infty(\mathbb{R}^+,\mathbb{C}^2)\,.$$

Thus, (5.1.21) defines a densely defined and symmetric operator on the Hilbert space (5.1.18) and the overall problem of the self-adjoint realisation of H is reduced to the same problem in each reducing subspace.

In particular, it is of physical relevance to consider each operator

$$h_{m_j} := h_{m_j,\kappa_j=j+\frac{1}{2}} \oplus h_{m_j,\kappa_j=-(j+\frac{1}{2})} \tag{5.1.22}$$

acting block-diagonal-wise, with the two different spin-orbit components, on the Hilbert eigenspace $L^2(\mathbb{R}^+,\mathbb{C}^4,\mathrm{d}r)$ of (j,m_j)-eigenvalue for J^2 and J_3.

Now, the following property is well known, as one can see by means of standard limit-point limit-circle arguments (see Section 1.4). Its proof is discussed in Section 5.3.1 where we compute deficiency indices for the operator H and every $\nu \in \mathbb{R}$.

Proposition 5.1.2. *The operator h_{m_j,κ_j} is essentially self-adjoint on its domain with respect to the Hilbert space $\mathcal{H}_{m_j,\kappa_j}$ if and only if*

$$\nu^2 \leqslant \kappa_j^2 - \tfrac{1}{4}\,, \tag{5.1.23}$$

and it has deficiency indices $(1,1)$ otherwise. In particular, in the regime $|\nu| \in (\frac{\sqrt{3}}{2},1)$ only the operators of the decomposition (5.1.20) with $\kappa_j^2 = 1$, thus

$$h_{\frac{1}{2},1}\,, \quad h_{-\frac{1}{2},1}\,, \quad h_{\frac{1}{2},-1}\,, \quad h_{-\frac{1}{2},-1}\,, \tag{5.1.24}$$

have deficiency indices $(1,1)$, all others being essentially self-adjoint.

Therefore the operator $h_{\frac{1}{2},1} \oplus h_{\frac{1}{2},-1} \oplus h_{-\frac{1}{2},1} \oplus h_{-\frac{1}{2},-1}$, and hence H itself, has deficiency indices $(4,4)$. This means that there is a 16-real-parameter family of self-adjoint extensions of H, hence of physically inequivalent realisations of the Dirac-Coulomb Hamiltonian. From the operator-theoretic point of view, the analysis of the self-adjoint extensions of $h_{\frac{1}{2},1}$ is the very same as for the other three operators (and in fact $h_{\frac{1}{2},1}$ and $h_{-\frac{1}{2},1}$ have the same formal action on $L^2(\mathbb{R}^+,\mathbb{C}^2)$, and so have $h_{\frac{1}{2},-1}$ and $h_{-\frac{1}{2},-1}$), and hence we will discuss only the first case.

There is room for extensions only on the sector $j = \frac{1}{2}$ of lowest total angular momentum J^2 and, as we shall discuss in Section 5.3, each extension corresponds to a particular prescription on the wave functions of the domain in the vicinity of the centre $x = 0$ of the Coulomb interaction. For higher j's the large angular momentum makes the Coulomb singularity lesser and lesser relevant, and on such sectors H is already essentially self-adjoint.

Physically, the relevant class of extensions is rather the *one*-parameter sub-family consisting of the same extension for each elementary operators (5.1.24), in a sense that will be evident in the next Section, that is, extensions where the same boundary conditions of self-adjointness occurs on each block of H – it would be non-physical to have a different behaviour of the physical Hamiltonian on different sectors $\mathcal{H}_{m_j, \kappa_j}$ of its symmetry.

A complete classification of the 'non physical' extensions, and the properties of their discrete spectra, is not present in the literature.

We would like to informally present at this point of the introductory section the result concerning the classification of self-adjoint extensions that will be rigorously proved in Section 5.3.

Theorem 5.1.3 (Classification of Dirac-Coulomb extensions – informal version). *Let* $|\nu| \in (\frac{\sqrt{3}}{2}, 1)$.

(i) *On each of the four sectors* $(j, m_j, k_j) = (\frac{1}{2}, \pm\frac{1}{2}, \pm 1)$ *of non-self-adjointness, the operator* H *admits a one-parameter family* $(S_\beta)_{\beta \in \mathbb{R} \cup \{\infty\}}$ *of self-adjoint extensions – which are then restrictions of* H^*.

(ii) *Whereas the domain of* H^* *in each sector consists of spinors g with* H^1-*regularity on* $[\varepsilon, +\infty)$ *for all* $\varepsilon > 0$ *and the short-distance asymptotics*

$$g(r) = g_0 r^{-\sqrt{1-\nu^2}} + g_1 r^{\sqrt{1-\nu^2}} + o(r^{1/2}) \quad as \ r \downarrow 0 \tag{5.1.25}$$

for some $g_0, g_1 \in \mathbb{C}^2$ *dependent on* ν *only, the domain* $\mathcal{D}(S_\beta)$ *of the extension* S_β *consists of those such spinors for which a prescribed ratio holds between the corresponding components of* g_1 *and* g_0, *for concreteness*

$$\frac{g_1^+}{g_0^+} = c_{\nu,\kappa}\,\beta + d_{\nu,\kappa} \tag{5.1.26}$$

for some explicitly known constants $c_{\nu,\kappa}, d_{\nu,\kappa} \in \mathbb{C}$.

(iii) *The extension* $\beta = \infty$ *is the restriction* S_D, *on the considered sector* (j, m_j, k_j), *of the distinguished extension* H_D *of H discussed in Theorem 5.1.1(ii): the functions in its domain have the asymptotics* (5.1.25) *with* $g_0 \equiv 0$, *i.e., without singular term.*

(iv) *All those extensions* S_β *with* $\beta \neq 0$ *are invertible with everywhere defined and bounded inverse, in which case the inverse* S_β^{-1} *is an explicit rank-one perturbation of* S_D^{-1}.

(v) *The gap in the spectrum of* S_β *around* $\lambda = 0$ *has a direct estimate in terms of* β *and* $\|S_D^{-1}\|$ *and must be at least the interval*

$$(-E_0(\beta), E_0(\beta)), \qquad E_0(\beta) := \frac{|\beta|}{|\beta|\|S_D^{-1}\| + 1}. \tag{5.1.27}$$

Our Theorem 5.1.3 provides a classification of the whole family of self-adjoint realisations of h which turns out to provide the appropriate scheme for qualifying the discrete spectrum of the generic extension h_β. In fact, we observe that our paper [48] stands in a gap in the literature between the well-established knowledge on the one hand that for critical couplings the Dirac-Coulomb Hamiltonian admits an infinite multiplicity of self-adjoint realisations, and the availability on the other hand of an eigenvalue formula for the distinguished extension only.

First, the natural question arises why the 'classical' methods for the determination of Sommerfeld's formula, mainly the ODE/truncation-of-series approach and the supersymmetric approach, did not determine other than the eigenvalues of the *distinguished* extension. We address this point in Section 5.4, exhibiting the precise steps of such classical methods in which one naturally selects only the discrete spectrum of the distinguished (and in fact also of a 'mirror' distinguished) realisation.

It actually turns out that there are no explicit alternatives: indeed, in the ODE approach to the differential eigenvalue problem the only alternative to truncating series is to deal with eigenfunctions expressed by infinite series, and imposing the eigenfunction with eigenvalue E to belong to some domain $\mathcal{D}(h_\beta)$ does not produce a closed formula for E any longer; on the other hand, in the supersymmetric approach the first order differential eigenvalue problem is studied by an auxiliary second order differential problem whose solutions only exhibit the boundary condition typical of the distinguished (or also of the 'mirror' distinguished) extension, with no access to different boundary conditions.

Next, we address the issue of how the eigenvalue formula (5.1.12), valid for $\beta = \infty$, gets modified for a generic extension parameter β. Our result is the following.

Theorem 5.1.4. *Let $k = \kappa_j \in \{\pm 1\}$ and let $(h_\beta)_{\beta \in (-\infty,\infty]}$ be the family of self-adjoint realisations, in the critical regime $|\nu| \in (\frac{\sqrt{3}}{2}, 1)$ of the Dirac-Coulomb Hamiltonian $h = h_{m_j, \kappa_j}$ defined in (5.1.21), according to the parametrisation given by Theorem 5.1.3. The discrete spectrum of a generic realisation h_β consists of the countable collection*

$$\sigma_{\mathrm{disc}}(h_\beta) \;=\; \big\{ E_n^{(\beta)} \,|\, n \in \mathbb{N}_0 \,, n \geqslant n_0 \big\} \;\subset\; (-1, 1) \tag{5.1.28}$$

of eigenvalues $E_n^{(\beta)}$ which are all the possible roots, enumerated in decreasing order when $\nu > 0$ and in increasing order when $\nu < 0$, of the transcendental equation

$$\mathfrak{F}_{\nu,k}(E_n^{(\beta)}) \;=\; c_{\nu,k}\,\beta + d_{\nu,k}\,, \tag{5.1.29}$$

where the constants $c_{\nu,k}$ and $d_{\nu,k}$ are the same as in Theorem 5.1.3.

$$\mathfrak{F}_{\nu,k}(E) \;:=\; \big(2\sqrt{1-E^2}\big)^{2\sqrt{1-\nu^2}}\, \frac{\Gamma(-2\sqrt{1-\nu^2})}{\Gamma(2\sqrt{1-\nu^2})}\, \frac{\nu\sqrt{\frac{1-E}{1+E}} + k - \sqrt{1-\nu^2}}{\nu\sqrt{\frac{1-E}{1+E}} + k + \sqrt{1-\nu^2}} \;\times$$
$$\times\; \frac{\Gamma\big(\frac{\nu E}{\sqrt{1-E^2}} + \sqrt{1-\nu^2}\big)}{\Gamma\big(\frac{\nu E}{\sqrt{1-E^2}} - \sqrt{1-\nu^2}\big)}\,. \tag{5.1.30}$$

The starting index of the enumeration is $n_0 = 0$ if k and ν have the same sign, and $n_0 = 1$ otherwise.

Equation (5.1.29) of Theorem 5.1.4, that will be proved in Section 5.5, provides the implicit formula for the eigenvalues of the generic extension h_β. A formula of the eigenfunctions corresponding to the eigenvalues $E_n^{(\beta)}$ is found in the proof of Theorem 5.1.4 – see (5.5.6) in Section 5.5.

In particular, equation (5.1.29) contains Sommerfeld's formula for the distinguished extension of h, namely the extension with $\beta = \infty$. For a comparison with the existing literature, let us formulate the latter consequence for generic $k \in \{\pm 1\}$.

Corollary 5.1.5. *Under the assumptions of Theorem 5.1.4, let h_D be the distinguished (i.e., $\beta = \infty$) self-adjoint extension of h. Then the eigenvalues $(E_n)_{n=n_0}^{\infty}$ of h_D are given by*

$$E_n \;=\; -\operatorname{sign}(\nu)\left(1 + \frac{\nu^2}{(n + \sqrt{1-\nu^2})^2}\right)^{-1/2}, \tag{5.1.31}$$

the starting index of the enumeration being $n_0 = 0$ if k and ν have the same sign, and $n_0 = 1$ otherwise.

The first five eigenvalues $E_0^{(\beta)}, \ldots, E_4^{(\beta)}$ for generic β are plotted in Figure 5.1 for the concrete case $k = 1$, $\nu > 0$. We obtained this plot by computing numerically the intersection points of the curve $E \mapsto \mathfrak{F}_{\nu,k}(E)$ with horizontal lines corresponding to various values of $c_{\nu,k}\,\beta + d_{\nu,k}$. In this case when $\beta > 0$ all eigenvalues are strictly negative (and accumulate to -1), whereas for a region of negative β's the first eigenvalue is positive. As to be expected, $E_0^{(\beta)} = 0$ only for $\beta = 0$: this corresponds to the sole non-invertible extension.
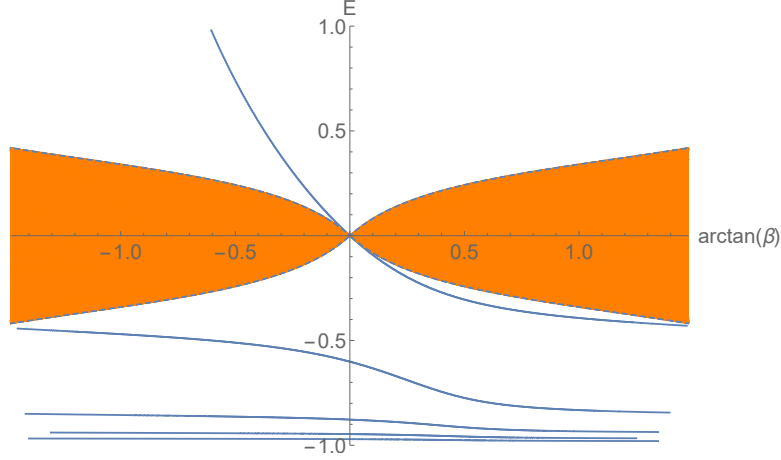

Figure 5.1: Numerical computation of the eigenvalues $E_n^{(\beta)}$ as functions of β, for $k = 1$ and $\nu = 0.9$. The shaded area is the region $|E| < E(\beta)$, with $E(\beta)$ given by (5.1.27), and indicates the estimated gap in the spectrum around zero, according to Theorem 5.1.4(vi).
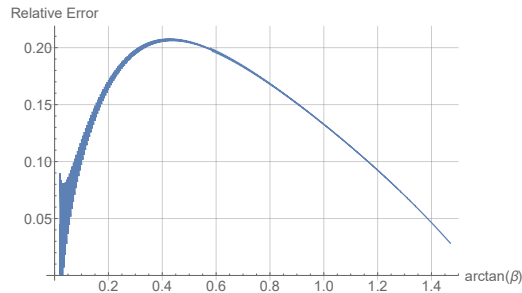

Figure 5.2: Relative error on the estimate of the ground state energy for positive β, in the case $k = 1$ and $\nu = 0.9$. The worse relative error is reached for $\beta \sim 0.58$ and amounts to about 20%.

It follows from the detailed discussion of the behaviour of $\mathfrak{F}_{\nu,k}(E)$ (in particular, of the vertical asymptotes of $\mathfrak{F}_{\nu,k}(E)$) which we are going to develop in Section 5.5 that each $E_n^{(\beta)}$ is smooth and strictly monotone in β, and it moves with continuity from $\beta = (+\infty)^-$ to $\beta = (-\infty)^+$. This results in a typical *fibred structure* of the union of all the discrete spectra $\sigma_{\mathrm{disc}}(h_\beta)$, with

$$\bigcup_{\beta \in (-\infty, +\infty]} \left\{ E_n^{(\beta)} \,|\, n \in \mathbb{N}_0 \,, n \geqslant n_0 \right\} \;=\; (-1, 1)\,. \tag{5.1.32}$$

Let us conclude the presentation of our results with a comment on the accuracy of the estimate (5.1.27) on the width of the spectral gap around zero for a generic extension h_β. Let us choose for

concreteness $k = 1$ and $\nu > 0$: the estimated gap in this case is superimposed in Figure 5.1 and turns out to be asymptotically exact for $\beta \to 0$ and $\beta \to +\infty$, and reasonably precise in between. Owing to Corollary 5.1.5 we can now write

$$\|h_D^{-1}\| \;=\; B^{-1} \;=\; (1 - \nu^2)^{-\frac{1}{2}} \,. \tag{5.1.33}$$

Thus, from (5.1.27) and (5.1.33) we conclude that

$$\mathcal{E}_0^{(\beta)} \;:=\; \frac{|\beta|}{1 + |\beta|(1 - \nu^2)^{-\frac{1}{2}}} \tag{5.1.34}$$

provides a good estimate (from below) of the *otherwise not explicitly computable* ground state $E_0^{(\beta)}$ of the generic self-adjoint extension h_β.

   Here is how the material of the section is organised. As mentioned already we start by a brief historical review of the problem in Section 5.2. In Section 5.3 we state rigorously our main results, whose proof, outlined in Section 5.3 itself, is based on intermediate results that we prove in Subsections 5.3.2, 5.3.3, and 5.3.4. In Subsection 5.3.1 we compute the deficiency indices and in Subsection 5.3.5 we discuss further properties of the Dirac-Coulomb extensions involving the resolvent and the spectral gap at zero. In Section 5.4 we revisit the classical methods used for computing an explicit formula for the eigenvalues of the Dirac-Coulomb operator and in Section 5.5 we compute the implicit formula for the spectrum of the generic extension by means of ODE methods.

   Last, we want to point out that Proposition 5.3.3 (and its proof in Subsection 5.3.4) contains a characterisation of the domain of the closure which is more complete with respect to the one we gave in [50].

5.2   Essential self-adjointness and the Distinguished extension

In this section we review the historical path that led to the present understanding on the existence and uniqueness of self-adjoint extensions of the minimal Dirac-Coulomb operator.

   Conceptually and historically the two main questions addressed so far, and that we are going to analyse are:

1. Is the operator $H_0 + V$ essentially self-adjoint?

2. If it is not, is there a *special* self-adjoint extension which is physically relevant?

   The technique employed in answering the first question is essentially a perturbative argument based on the Kato-Rellich theorem and it is addressed in the first subsection.

   The second question presents a wider range of answers and many authors provided different meaningful special extensions. Only at a later stage they recognized that, under some hypothesis, they were referring to the same operator. This subject is addressed in the second subsection.

5.2.1   Essential self-adjointness via Kato-Rellich theorem

One of the first proofs of the essential self-adjointness for the Dirac-Coulomb operator is due to Kato in 1951 as a direct application of the Kato-Rellich theorem. Despite the simplicity of the proof, this does not cover the whole range of the parameter ν on which the Dirac-Coulomb operator is essentially self-adjoint.

   Some years later two different approaches based on the same theorem were developed in order to cover the range $[0, \frac{\sqrt{3}}{2}]$: the first one, due to Rejtö and Gustafsson [97, 61] aimed to weaken its hypotheses, the other one due to Schminke [103] uses the original theorem. Instead of looking to V

as a perturbation of H_0 he introduced an operator C and considered $H_0 + V = (H_0 + C) + (V - C)$. To prove the essential self-adjointness of $H_0 + V$ he proved separately the essential self-adjointness of $H_0 + C$ and looked at $V - C$ as a perturbation satisfying the hypothesis of Kato-Rellich.

Several other works dealt with the same problem, among which we mention [99, 101, 42, 117, 28, 77]. For a self-contained conceptual review we present in detail only the above-mentioned ones of Rejtö-Gustaffson and Schmincke.

Since it will play a central role in this subsection, we recall the classical statement of the Kato-Rellich theorem (as stated in [95, Theorem X.12]).

Theorem 5.2.1 (Kato-Rellich). *Suppose that A is an essentially self-adjoint operator, B is a symmetric operator that is A-bounded with relative bound $a < 1$, namely*

i) $\mathcal{D}(B) \supset \mathcal{D}(A)$;

ii) For some $a < 1$, $b \in \mathbb{R}$ and for all $\varphi \in \mathcal{D}(A)$,

$$\|B\varphi\| \leqslant a\|A\varphi\| + b\|\varphi\|. \tag{5.2.1}$$

Then $\overline{A + B}$ is self-adjoint on $\mathcal{D}(\overline{A})$ and essentially self-adjoint on any core of A.

Let us start with surveying Kato's proof from [69, 71]. The starting point is the well-known Hardy inequality (see [95] section X.2 p.169)

$$\|\boldsymbol{p}u\|^2 \geqslant \frac{1}{4}\|r^{-1}u\|^2, \qquad \forall u \in C_c^\infty(\mathbb{R}^3). \tag{5.2.2}$$

By using the ancticommutation properties of the $\boldsymbol{\alpha}$ matrices we get the identity

$$\|H_0 u\|^2 = \|\boldsymbol{p}u\|^2 + \langle (\beta\boldsymbol{\alpha} \cdot \boldsymbol{p} + \boldsymbol{\alpha} \cdot \boldsymbol{p}\beta)u, u\rangle + \|u\|^2 = \|\boldsymbol{p}u\|^2 + \|u\|^2. \tag{5.2.3}$$

Thus, we see that if the potential is $|\phi(x)| \leqslant \frac{\nu}{|x|}$, we get the following chain of inequalities

$$\|\boldsymbol{p}u\|^2 \geqslant \frac{1}{4}\|r^{-1}u\|^2 \geqslant \frac{1}{4\nu^2}\|\phi(x)u\|^2, \tag{5.2.4}$$

from which it follows that

$$\|\phi(x)u\| \leqslant 4\nu^2\|H_0 u\|^2 - 4\nu^2\|u\|^2. \tag{5.2.5}$$

If $\nu < \frac{1}{2}$, the hypotheses of the Kato-Rellich theorem are satisfied and one deduces that $H_0 + V$ is essentially self-adjoint and the domain of the unique self adjoint extension is

$$\mathcal{D}(\overline{H_0 + V}) = H^1(\mathbb{R}^3) \otimes \mathbb{C}^4. \tag{5.2.6}$$

Remark 5.2.2. By using Wüst theorem (see [95] theorem X.14) one can cover the case $\nu = \frac{1}{2}$. However the information on the domain of the self-adjoint extension is lost.

Remark 5.2.3. The result is independent of the possible spherical symmetry and of precise matricial form of the potential: the conclusion holds if $\lim_{x\to 0} |x||V_{ij}(x)| < \frac{1}{2}$, where $i, j = 1, 2$ and V_{ij} are the entries of the matrix V.

Remark 5.2.4. Arai [7, 8] showed that by considering more general matrix-valued potentials of the form

$$V(x) = \frac{Z}{r}\mathbb{1} + \frac{\mathrm{i}}{r}\boldsymbol{\alpha} \cdot \hat{\boldsymbol{r}}\beta b_1 + \frac{\beta}{r}b_2 \tag{5.2.7}$$

the necessary and sufficient condition for the essential self-adjointness is $(\kappa_j + b_1)^2 + b_2^2 \geqslant Z^2 + \frac{1}{4}$ and hence the threshold $\frac{1}{2}$ is optimal, in the sense that if V is in the form above and one of the entry of the matrix satisfies $|x||V_{ij}| > \frac{1}{2}$ then it is possible to choose Z, b_1, b_2 such that the operator is not essentially self-adjoint.

In a work of 1970, Rejtö [97] discussed the particular case of spherically symmetric Coulomb-like potentials. By denoting with $B(\mathcal{H})$ the set of bounded operators on $\mathcal{H}$, the requirement on V for the operator $H_0 + V$ to be essentially self-adjoint on $C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)$ boils down to asking that $\exists \mu_\pm$ in the upper/lower closed complex half plane such that

$$(\mathbb{1} - \overline{V}(\mu_\pm - \overline{H_0})^{-1}) \in B(\mathcal{H}). \tag{5.2.8}$$

Proving that the Dirac operator with Coulomb interaction satisfies this hypothesis for $\nu \in [0, \frac{3}{4})$, he was able to show that under this condition such an operator is essentially self-adjoint and the domain of its self-adjoint extension is $H^1(\mathbb{R}^3) \otimes \mathbb{C}^4$.

In fact [97] provides some sort of intermediate results that led to the more relevant work [61] by Gustaffson and Rejtö. In this relevant follow-up work they generalised further Kato-Rellich theorem and they were able to achieve the essential self-adjointness for the Dirac operator in the regime $\nu \in [0, \sqrt{3}/2)$.

Their generalisation relies on Fredholm's theory, that we briefly recall here for the self-consistency of the presentation. A densely defined operator A in a Banach space $\mathcal{X}$ is said to be Fredholm if A is closed, ran A is closed, and both $\dim \ker A$ and $\dim \mathcal{X}/\operatorname{ran} T$ are finite. The index of a Fredholm operator A is the number $i(T) = \dim \ker A - \dim \mathcal{X}/\operatorname{ran} A$.

Theorem 5.2.5 ([61], Theorem 3.1, Generalised Kato-Rellich theorem). *Let H_0 be essentially self-adjoint, V symmetric with $\mathcal{D}(V) \supset \mathcal{D}(H_0)$ where V is H_0-bounded. For each μ in the resolvent set of H_0 define the operator $A_\mu \in B(\mathcal{H})$ by*

$$A_\mu := \mathbb{1} - \overline{V}(\mu - \overline{H_0})^{-1}. \tag{5.2.9}$$

Then the three conditions below

i) $H_0 + V$ is essentially self-adjoint;

ii) $\overline{H_0 + V} = \overline{H_0} + \overline{V}$;

iii) $\mathcal{D}(\overline{H_0 + V}) = \mathcal{D}(\overline{H_0})$;

hold if and only if there exists μ_+ in the closed upper half plane and μ_- in the closed lower half plane such that the operators $A_{\mu_\pm}$ are Fredholm of index zero.

Proof. (Sketch) We start from the identity

$$\mu - \overline{H_0} - \overline{V} = [\mathbb{1} - \overline{V}(\mu - \overline{H_0})^{-1}](\mu - \overline{H_0}). \tag{5.2.10}$$

Since $\mu \in \rho(H_0)$, $\mu - \overline{H_0}$ is Fredholm of index zero and since the composition of Fredholm operators is Fredholm and the index of the composition is the sum of the indices, by using a standard criterion of essential self-adjointness, we prove the sufficient condition.

The necessity follows using the same index-formula and the fact that if $A_1 A_2$ is Fredholm with A_2 Fredholm and A_1 closed, then A_1 is Fredholm and therefore by the above formula $A_{\pm i}$ is Fredholm of index 0. □

Remark 5.2.6. This theorem includes the classical Kato-Rellich noting that with $\mu_\pm = \pm i \frac{a}{b}$ one has $\|\overline{V}(\mu_\pm - \overline{H_0})^{-1}\| < 1$. Hence $A_{\mu_\pm}$ are invertible and therefore Fredholm of index zero.

The proof of the essential self-adjointness of the Dirac operator with Coulomb potential uses the following corollary:

Corollary 5.2.7. *If there exist μ_+ and μ_- as in the previous theorem such that $A_{\mu_\pm} = B_\pm + C_\pm$ where $B_\pm^{-1} \in B(\mathcal{H})$ and $C_\pm$ are compact, then $H_0 + V$ is essentially self-adjoint and $\mathcal{D}(\overline{H_0 + V}) = \mathcal{D}(\overline{H_0})$.*

Proof. This corollary follows from the fact that an invertible operator is Fredholm of index zero and that this property is stable under compact perturbations. $\qquad \square$

By using the spherical symmetry and the decomposition of the Dirac operator Rejtö and Gustaffson prove that for $|\nu| \in [0, \frac{\sqrt{3}}{2})$ the hypothesis of Corollary 5.2.7 are satisfied and hence the spherically symmetric Dirac-Coulomb operator is essentially self-adjoint for that range of parameters.

In this respect the work of Schmincke [103] is of interest in that the same conclusion on essential self-adjointness was obtained *independently* of the spherical symmetry of the potential.

Theorem 5.2.8 ([103]). *Let $\phi \in L^2_{loc}(\mathbb{R}^3 \setminus \{0\})$ be a real-valued function that can be expressed as $\phi = \phi_1 + \phi_2$ with $\phi_1 \in C^0(\mathbb{R}^3 \setminus \{0\})$ and $\phi_2 \in L^\infty(\mathbb{R}^3 \setminus \{0\})$ with*

$$|\phi_1(x)| \leqslant \frac{\nu}{|x|} \tag{5.2.11}$$

and $\nu \in [0, \frac{\sqrt{3}}{2})$. Then $H_0 + V$ is essentially self-adjoint.

The way Schmincke proves its result consists of using the standard Kato-Rellich theorem. He introduces a certain intercalary operator C in order to write $H_0 + V = (H_0 + C) + (V - C)$ and to regard $V - C$ as a small perturbation of $H_0 + C$.

After setting

$$C := \frac{1}{4}\left(a - \frac{1}{r}\right)\boldsymbol{\alpha} \cdot \hat{\boldsymbol{r}}, \qquad 1 < a < 3 \tag{5.2.12}$$

and $H_0 = \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta$, he introduces a bounded operator S_2 on which we omit the details. From these definitions it is clear that for $z \in \mathbb{C}$, $0 < |z| < 1$,

$$H_0 + V = (A + \beta + zC) + (V - zC - S_2) + S_2 = F + G + S_2. \tag{5.2.13}$$

With these definitions Schmincke proves that $\|Gu\|^2 \leqslant k\|Fu\|^2$ with $k < 1$ and hence Gu is F-bounded with a small bound. One can thus apply Kato-Rellich[1] to obtain that $T + V + S_2$ is essentially self-adjoint and, since S_2 is a bounded operator, this also implies the essentially self-adjointness of T.

5.2.2 The distinguished self-adjoint extension

As stated in Theorem 5.1.1, in the critical regime there are infinitely many self-adjoint extensions of the minimal Dirac-Coulomb operator. Before considering their classification the main interest throughout the 1970s was the study of a *distinguished* extension characterized by being the most physically meaningful. The first work that introduced this particular self-adjoint extension is due to Schmincke [102] who obtained this extension by means of a multiplicative intercalary operator. This self-adjoint realisation is physically relevant because its domain is contained in the domain of the potential energy form and hence each function on the domain has a finite expectation value of the potential energy operator.

A second and more explicit construction of a distinguished self-adjoint extension of the minimal Dirac-Coulomb operator was found by Wüst [122, 123] by means of cut-off potentials. He built a sequence of self-adjoint operators that converges strongly in the operator graph topology to a self-adjoint extension of the minimal Dirac-Coulomb operator. Remarkably that the domain of this self-adjoint extension is also contained in the domain of the potential energy.

At that point it was not clear whether Wüst's and Schmincke's self-adjoint extensions were the same or not. The first attempt to look for a distinguished self-adjoint extension with a requirement

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[1]Schmincke used a complex version of Kato-Rellich that deals with closed operators instead of self-adjoint ones. This is necessary because, in general, the z appearing in the proof is not real.

of uniqueness was made by Nenciu [89] who found that there exists a unique self-adjoint extension of the minimal Dirac operator whose domain is contained in the domain of the kinetic energy form.

In 1979 Klaus and Wüst [72] proved that in the regime $\nu \in (\frac{\sqrt{3}}{2}, 1)$ if the potential ϕ is semi-bounded all the above mentioned distinguished self-adjoint extensions coincide.

Let us start with Schmincke's result.

Theorem 5.2.9 ([102], Theorems 2 and 3). *Let $\phi \in L^2_{loc}(\mathbb{R}^3 \setminus \{0\}, \mathbb{R}, \mathrm{d}x)$ be a real-valued function such that $\phi = \phi_1 + \phi_2$ with ϕ_1 and ϕ_2 both real valued, $\phi_1 \in C^0(\mathbb{R}^3 \setminus \{0\})$, and $\phi_2 \in L^\infty(\mathbb{R}^3, \mathbb{R}, \mathrm{d}x)$. Let $s \in [0, 1)$. Suppose there exists $k > 1$, $c > 1$ and $f \in C^1((0, \infty))$ positive valued and bounded from above by $\frac{1-s}{2c}$ such that*

$$\frac{1}{r^2}\left(f(r) + \frac{s}{2}\right)^2 \leqslant k\left(|\phi_1(x)|^2 + \frac{1}{r^2}f^2(r)\right) \leqslant$$
$$\leqslant \frac{1}{r^2}\left(f(r) + \frac{s+1}{2}\right)^2 + \frac{1}{r}f'(r). \tag{5.2.14}$$

Then there exists a bounded symmetric operator S such that

$$H_G := \left(\overline{r^{-\frac{s}{2}}}\right)\left(\overline{r^{\frac{s}{2}}(H - S)}\right) + \overline{S} \tag{5.2.15}$$

is an essential self-adjoint extension of H and $\forall m \in [\frac{1}{2}, 1 - \frac{s}{2}]$

$$\mathcal{D}(H_G) = \mathcal{D}(H^*) \cap \mathcal{D}\left(\overline{r^{-m}}\right). \tag{5.2.16}$$

Remark 5.2.10. Note that in particular $\mathcal{D}(H_G) \subset \mathcal{D}\left(\overline{r^{-1/2}}\right)$, which physically means that all the functions in the domain of this distinguished self-adjoint extension have a finite expectation of the potential energy.

Schmincke proved this using a multiplicative intercalary operator. If $T = H_0 + V$ with H_0 essentially self-adjoint and if there exists a symmetric operator G satisfying suitable properties (see Theorem 1 in [102]), then

$$H_G := \overline{G^{-1}}\,\overline{GH} \tag{5.2.17}$$

is an essentially self-adjoint extension of H.

Noticeably in the case of Coulomb potential the assumptions of the theorem are satisfied when

$$1 - 4\nu^2 \leqslant (1 - s^2) \leqslant 4(1 - \nu^2), \tag{5.2.18}$$

which means $\nu < 1$.

Wüst, instead, showed that given a potential $\phi(x) \in C^0(\mathbb{R}^3 \setminus \{0\})$ such that

$$|\phi(x)| \leqslant \frac{\nu}{|x|} \qquad |\nu| < 1, \tag{5.2.19}$$

if one fixes a positive constant $c > 0$ and defines

$$V_t(x) := \begin{cases} V(x) & |x| \geqslant \frac{c}{t} \\ R(x) & |x| < \frac{c}{t}, \end{cases} \tag{5.2.20}$$

where R is chosen such that the components of H_t are continuous functions. If $H_t(x)$ is definitely monotone, the sequence of operators $T_t = H_0 + V_t$ g-converges to a self-adjoint operator H_g which is a self-adjoint extension of H with the property that

$$\mathcal{D}(H_g) \subset \mathcal{D}\left(\overline{r^{1/2}}\right). \tag{5.2.21}$$

In 1976 Nenciu [89] proposed an alternative distinguished self-adjoint extension H_N by requiring this extension to be the unique with the property that all the functions in its domain have finite kinetic energy, namely

$$\mathcal{D}(H_N) \subset \mathcal{D}(|\overline{H_0}|^{\frac{1}{2}}). \tag{5.2.22}$$

The precise result can be stated as follows.

Theorem 5.2.11 ([89], Theorem 5.1)**.** *Let $w(t)$ be a decreasing function on $[0, \infty)$ such that $0 \leqslant w(t) \leqslant 1$, $\lim_{t\to\infty} w(t) = 0$, H_0 and V be a matrix-valued potential.*
If

i) *$V(x) = w(|x|)W(x)$ where W is a small perturbation of H_0, or*

ii) *$V(x) = V_1(x) + V_2(x)$ where V_1 is dominated by the Coulomb potential with coupling constant $\nu < 1$ and $V_2 = w(|x|)W_2(x)$ where W_2 is non-singular,*

then

i) *there exists a unique operator H_N such that*

$$\mathcal{D}(H_N) \subset \mathcal{D}(|\overline{H}_0|^{\frac{1}{2}}); \tag{5.2.23}$$

ii) *$\sigma_{ess}(H) \subset \sigma_{ess}(H_0)$.*

The proof relies on a variant of Lax-Milgram lemma and has the inconvenience not to be constructive.

In 1979 Klaus and Wüst [72] showed that in the case of semi-bounded potential Wüst's and Nenciu's distinguished extensions actually coincide. This is an interesting fact both from a physical and from a mathematical point of view. Physically this coincidence means that the distinguished self-adjoint extension has the property of being the only one whose functions in the domain have finite potential *and* kinetic energy. From a mathematical point of view this overcomes the fact that Nenciu's method was not constructive and provides instead an explicit expression for its self-adjoint extension in terms of g-limit of H_t.

The identification of a certain *distinguished extension* was pushed further by Esteban and Loss [41] up to the value $\nu = 1$. In that paper they proposed to define the distinguished self-adjoint extension via Hardy-Dirac inequalities. By a limit argument this procedure can define a sort of distinguished self-adjoint extension also when $\nu = 1$ but, in that case, the domain of this self-adjoint extension will be neither contained in the domain of the kinetic energy form nor in the domain of the potential energy form. In a subsequent work, Arrizabalaga [10] weakened further the hypothesis on the construction of the self-adjoint extension of Esteban and Loss.

5.3 Self-adjoint realisations and classification

The original Kreĭn-Višik-Birman scheme for the determination and classification of the self-adjoint extensions of a given densely defined and symmetric operator on Hilbert space was developed for *semi-bounded* operators: for this case one can non-restrictively assume that the bottom of the operator S to extend is strictly positive and hence a canonical extension exists, the Friedrichs extension S_F, with the same bottom and hence with everywhere defined bounded inverse S_F^{-1}.

In fact, to a large extent, the role of S_F in the theory can be played as well by any other 'distinguished' self-adjoint extension S_D of S which is itself invertible with everywhere defined and bounded inverse S_D^{-1}, and this makes many results of the theory applicable also to a (densely defined and symmetric) non-semi-bounded S, provided that S admits such an extension S_D. In this spirit, Grubb's 'universal classification' scheme was later developed [58] (a modern survey of which may be

found in [60, Chapter 13]), which only makes reference to the existence of an invertible extension and, in the case of symmetric operators, it reproduces many features of the Kreĭn-Višik-Birman scheme.

When applying Theorem 2.2.1 to the extension problem for the operator h_{m_j,κ_j} defined in (5.1.21) on the Hilbert space $\mathcal{H}_{m_j,\kappa_j}$ defined in (5.1.18), it is natural that the reference extension is the distinguished extension of Theorem 5.1.1(ii).

Acting on the Hilbert space $L^2(\mathbb{R}^+,\mathbb{C}^2,\mathrm{d}r)$ with scalar product

$$\langle \psi, \phi \rangle_{L^2(\mathbb{R}^+,\mathbb{C}^2)} \;=\; \int_0^{+\infty} \langle \psi(r), \phi(r) \rangle_{\mathbb{C}^2} \,\mathrm{d}r \;=\; \sum_{\alpha=\pm} \int_0^{+\infty} \overline{\psi^\alpha(r)}\,\phi^\alpha(r)\,\mathrm{d}r$$
$$\psi \equiv \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix}, \, \phi \equiv \begin{pmatrix} \phi^+ \\ \phi^- \end{pmatrix} \;\in\; L^2(\mathbb{R}^+,\mathbb{C}^2)\,, \tag{5.3.1}$$

we consider the operator

$$S \;:=\; \begin{pmatrix} 1+\frac{\nu}{r} & -\frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{r} \\ \frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{r} & -1+\frac{\nu}{r} \end{pmatrix}, \tag{5.3.2}$$
$$\mathcal{D}(S) \;:=\; C_0^\infty(\mathbb{R}^+,\mathbb{C}^2)\,.$$

S is non-semi-bounded, densely defined, and symmetric, and following from Proposition 5.1.2 it has deficiency indices $(1,1)$. For convenience, let us also denote by $\widetilde{S}$ the differential operator defined by

$$\widetilde{S}\begin{pmatrix} f^+ \\ f^- \end{pmatrix} \;:=\; \begin{pmatrix} 1+\frac{\nu}{r} & -\frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{r} \\ \frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{r} & -1+\frac{\nu}{r} \end{pmatrix}\begin{pmatrix} f^+ \\ f^- \end{pmatrix}. \tag{5.3.3}$$

Since $\widetilde{S}$ has real smooth coefficients, and is formally self-adjoint, it is a standard fact (Lemma 1.2.3) that the operator closure $\overline{S}$ and the adjoint S^* of S are nothing but, respectively, the *minimal* and the *maximal realisation* of $\widetilde{S}$, that is, they both act as $\widetilde{S}$ respectively on

$$\mathcal{D}(\overline{S}) \;=\; \overline{C_0^\infty(\mathbb{R}^+,\mathbb{C}^2)}^{\|\cdot\|_S}$$
$$\mathcal{D}(S^*) \;=\; \{\psi \in L^2(\mathbb{R}^+,\mathbb{C}^2)\,|\,\widetilde{S}\psi \in L^2(\mathbb{R}^+,\mathbb{C}^2)\}\,, \tag{5.3.4}$$

where $\|\cdot\|_S$ is the graph norm associated with S. One has $\overline{S} \subset S^*$, and by *self-adjoint realisation* of S we shall mean any operator $R=R^*$ on $L^2(\mathbb{R}^+,\mathbb{C}^2)$ such that $\overline{S} \subset R \subset S^*$.

In order to identify the self-adjoint realisations of S using the Kreĭn-Višik-Birman scheme of Theorem 2.2.1, we shall collect the intermediate results of Propositions 5.3.1, 5.3.2, and 5.3.3 below, whose proof is deferred to the following Subsections.

For convenience, let us introduce the parameter

$$B \;:=\; \sqrt{1-\nu^2}\,. \tag{5.3.5}$$

It will be important to remember throughout our analysis that $B \in (0,\frac{1}{2})$.

First one needs a characterisation of $\ker S^*$.

Proposition 5.3.1. *For every* $|\nu| \in (\frac{\sqrt{3}}{2},1)$ *the operator* S^* *has a one dimensional kernel, spanned by the function*

$$\Phi \;=\; \begin{pmatrix} \Phi^+ \\ \Phi^- \end{pmatrix} \tag{5.3.6}$$

with

$$\Phi^\pm(r) \;:=\; e^{-r}r^{-B}\big(\tfrac{\pm(1+\nu)+B}{1+\nu}\,U_{-B,1-2B}(2r) - \tfrac{2rB}{1+\nu}\,U_{1-B,2-2B}(2r)\big)\,, \tag{5.3.7}$$

where $U_{a,b}(r)$ is the Tricomi function [1, Sec. 13.1.3]. Φ is analytic on $(0, +\infty)$ with asymptotics

$$
\begin{aligned}
\Phi(r) &= r^{-B} \frac{\Gamma(2B)}{\Gamma(B)} \begin{pmatrix} \frac{1+\nu+B}{1+\nu} \\ -\frac{1+\nu-B}{1+\nu} \end{pmatrix} + \begin{pmatrix} q^+ \\ q^- \end{pmatrix} r^B + O(r^{1-B}) \quad as \; r \downarrow 0 \\
\Phi(r) &= 2^B \begin{pmatrix} 1 \\ -1 \end{pmatrix} r^{-B} e^{-r} (1 + O(r^{-1})) \quad as \; r \to +\infty,
\end{aligned}
\tag{5.3.8}
$$

where $q^{\pm}$ are both non-zero and explicitly given by (5.3.43) below.

Next, one needs to identify a reference extension S_D of S which be self-adjoint and with everywhere defined inverse, and to characterise the action of S_D on $\ker S^*$.

Proposition 5.3.2.

(i) *There exists a self-adjoint realisation S_D of S with the property that*

$$
\mathcal{D}(S_D) \subset H^{1/2}(\mathbb{R}^+, \mathbb{C}^2) \quad or \quad \mathcal{D}(S_D) \subset \mathcal{D}[r^{-1}], \tag{5.3.9}
$$

where the latter is the form domain of the multiplication operator by r^{-1} on each component of $L^2(\mathbb{R}^+, \mathbb{C}^2)$ (the space of 'finite potential energy'). S_D is the only self-adjoint realisation of S satisfying (5.3.9).

(ii) *S_D is invertible on $L^2(\mathbb{R}^+, \mathbb{C}^2)$ with everywhere defined and bounded inverse. The* explicit *integral kernel of S_D is given by (5.3.53).*

(iii) *In terms of the spaces $\mathcal{D}(\overline{S})$ and $\ker S^*$ one has*

$$
\mathcal{D}(S_D) = \mathcal{D}(\overline{S}) \dotplus S_D^{-1} \ker S^*. \tag{5.3.10}
$$

Moreover,

$$
\begin{aligned}
\mathcal{D}(S^*) &= \mathcal{D}(S_D) \dotplus \ker S^*, \\
&= \mathcal{D}(\overline{S}) \dotplus S_D^{-1} \ker S^* \dotplus \ker S^*.
\end{aligned}
\tag{5.3.11}
$$

(iv) *For the vector $S_D^{-1}\Phi$, where $\Phi \in \ker S^*$ is given by (5.3.6)-(5.3.7), one has the following pointwise asymptotics:*

$$
S_D^{-1}\Phi(r) \sim \begin{pmatrix} p^+ \\ p^- \end{pmatrix} r^B + o(r^{1/2}) \quad as \; r \downarrow 0, \tag{5.3.12}
$$

where $p^{\pm}$ are both non-zero and explicitly given in (5.3.60) below.[2]

Last, an amount of information is needed on the domain of the operator closure $\overline{S}$ of S. This is the subject of Subsection 5.3.4 where we will present a complete characterisation of $\mathcal{D}(\overline{S})$, from which we will be able to deduce the following properties, relevant for our main results.

Proposition 5.3.3. *For $\nu \in (\frac{\sqrt{3}}{2}, 1)$, $\mathcal{D}(\overline{S}) = H_0^1(\mathbb{R}^+)$ and, in particular, if $f \in \mathcal{D}(\overline{S})$,*

$$
f(r) = o(r^{1/2}) \quad as \quad r \downarrow 0. \tag{5.3.13}
$$

With Propositions 5.3.1, 5.3.2, and 5.3.3 at hand, we can now formulate a general classification as follows.

---

[2]In fact, with a slightly more elaborate argument we can better estimate the reminder in (5.3.12) as a $O(r^{1-B})$ term; however, this is not needed in the analysis that follows.

Theorem 5.3.4 (Classification of the self-adjoint realisations for the Dirac-Coulomb Hamiltonian – structural version)**.**
The self-adjoint extensions of the operator S on $L^2(\mathbb{R}^+, \mathbb{C}^2, dr)$ defined in (5.3.2) constitute a one-parameter family $(S_\beta)_{\beta \in \mathbb{R} \cup \{\infty\}}$ of restrictions of the adjoint operator S^* determined in (5.3.4), each of which is given by

$$S_\beta := S^* \upharpoonright \mathcal{D}(S_\beta)$$

$$\mathcal{D}(S_\beta) := \left\{ g = f + c(\beta S_D^{-1}\Phi + \Phi) \,\middle|\, \begin{array}{l} f \in \mathcal{D}(\overline{S}) \\ c \in \mathbb{C} \end{array} \right\}. \tag{5.3.14}$$

Here S_D is the distinguished self-adjoint extension of S identified in Proposition 5.3.2 and Φ is the spanning element of $\ker S^*$ identified in Proposition 5.3.1. In this parametrisation the distinguished extension S_D corresponds to $\beta = \infty$. For each $g \in \mathcal{D}(S_\beta)$ the function $f \in \mathcal{D}(\overline{S})$ and the constant $c \in \mathbb{C}$ are uniquely determined.

Mirror to the parametrisation formula (5.3.14), we can re-express the above result in terms of boundary conditions at the centre of the Coulomb singularity.

Theorem 5.3.5 (Classification of the self-adjoint realisations for the Dirac-Coulomb Hamiltonian – boundary condition version)**.**

(i) *Any function $g = \begin{pmatrix} g^+ \\ g^- \end{pmatrix} \in \mathcal{D}(S^*)$ satisfies the short-distance asymptotics*

$$\lim_{r \downarrow 0} r^B g(r) = g_0$$

$$\lim_{r \downarrow 0} r^{-B}(g(r) - g_0 r^{-B}) = g_1 \tag{5.3.15}$$

for some $g_0, g_1 \in \mathbb{C}^2$. In particular,

$$g(r) = g_0\, r^{-B} + g_1 r^B + o(r^{1/2}) \qquad \text{as } r \downarrow 0. \tag{5.3.16}$$

(ii) *The self-adjoint extensions of the operator S on $L^2(\mathbb{R}^+, \mathbb{C}^2)$ defined in (5.3.2) constitute a one-parameter family $(S_\beta)_{\beta \in \mathbb{R} \cup \{\infty\}}$ of restrictions of the adjoint operator S^*, each of which is given by*

$$S_\beta := S^* \upharpoonright \mathcal{D}(S_\beta)$$

$$\mathcal{D}(S_\beta) := \left\{ g \in \mathcal{D}(S^*) \,\middle|\, \frac{g_1^+}{g_0^+} = c_\nu \beta + d_\nu \right\}, \tag{5.3.17}$$

where

$$c_\nu = p^+ \left(\frac{\Gamma(2B)}{\Gamma(B)} \frac{1+\nu+B}{1+\nu} \right)^{-1}$$

$$d_\nu = q^+ \left(\frac{\Gamma(2B)}{\Gamma(B)} \frac{1+\nu+B}{1+\nu} \right)^{-1}, \tag{5.3.18}$$

and p^+ and q^+ are given, respectively, by (5.3.60) and (5.3.43). This is precisely the same parametrisation of the extension as in Theorem 5.3.4.

The proofs of Theorems 5.3.4 and 5.3.5 are an application of the general Kreĭn-Višik-Birman Theorem 2.2.1, through the intermediate results of Propositions 5.3.1, 5.3.2, and 5.3.3, as we shall show in a moment. Owing to further corollaries of Theorem 2.2.1, which we work out in detail in Section 5.3.5 (Theorem 5.3.17 therein), we can supplement the above extension picture with

an additional amount of information concerning the invertibility, the resolvent, and the spectral gap of each realisation S_β. This too is an example of relevant and non-trivial features of the self-adjoint extensions that can be established in a relatively cheap and elementary manner, unlike the counterpart way based on von Neumann's extension theory.

Theorem 5.3.6 (Invertibility, resolvent, and estimate on the spectral gap)**.**
The elements of the family $(S_\beta)_{\beta \in \mathbb{R} \cup \{\infty\}}$ of the self-adjoint extensions of the operator S on $L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r)$ defined in (5.3.2), labelled according to the parametrisation of Theorem 5.3.4, have the following properties.

(i) *S_β is invertible on the whole $L^2(\mathbb{R}^+, \mathbb{C}^2)$ if and only if $\beta \neq 0$.*

(ii) *For each invertible extension S_β,*

$$S_\beta^{-1} = S_D^{-1} + \frac{1}{\beta \|\Phi\|^2} |\Phi\rangle\langle\Phi|. \tag{5.3.19}$$

(iii) *For each invertible extension S_β,*

$$\sigma_{\mathrm{ess}}(S_\beta) = \sigma_{\mathrm{ess}}(S_D) = (-\infty, -1] \cup [1, +\infty), \tag{5.3.20}$$

and the gap in the spectrum $\sigma(S_\beta)$ around $E = 0$ is at least the interval $(-E(\beta), E(\beta))$, where

$$E(\beta) := \frac{|\beta|}{|\beta| \|S_D^{-1}\| + 1}. \tag{5.3.21}$$

We conclude this Section with the proof of Theorems 5.3.4 and 5.3.5, and we defer the proof of the technical intermediate results and of Theorem 5.3.6 to the following Sections.

Proof of Theorem 5.3.4. One extension is surely the distinguished extension S_D, with domain $\mathcal{D}(S_D) = \mathcal{D}(\overline{S}) \dotplus S_D^{-1} \ker S^*$ (Proposition 5.3.2(iii)), which is of the form (5.3.14) for $\beta = \infty$: indeed, with respect to the general formula (2.2.1), this is the extension that corresponds to an operator T defined on $\{0\} \subset \ker S^*$. Since $\dim \ker S^* = 1$ (Proposition 5.3.1), for all other extensions of S the parametrising operator T, in the sense of the general formula (2.2.1), must be self-adjoint on the whole one-dimensional span$\{\Phi\}$, and therefore is the multiplication operator by a scalar β. Then (2.2.1) takes the form (5.3.14). The uniqueness of the decomposition of $g \in \mathcal{D}(S_\beta)$ into $g \in \mathcal{D}(S_\beta)$ is a direct consequence of the direct sum decomposition (5.3.11) of Proposition 5.3.2(iii). $\qquad \square$

Proof of Theorem 5.3.5.
(i) It was determined in Propositions 5.3.1, 5.3.2, and 5.3.3 that a generic $g \in \mathcal{D}(S^*)$ decomposes with respect to (5.3.11) as

$$\begin{pmatrix} g^+ \\ g^- \end{pmatrix} = \begin{pmatrix} f^+ \\ f^- \end{pmatrix} + a\, S_D^{-1} \begin{pmatrix} \Phi^+ \\ \Phi^- \end{pmatrix} + \frac{b}{\gamma} \begin{pmatrix} \Phi^+ \\ \Phi^- \end{pmatrix} \quad \gamma := \frac{\Gamma(2B)}{\Gamma(B)} \frac{1+\nu+B}{1+\nu} \tag{5.3.22}$$

for some $a, b \in \mathbb{C}$, and moreover, as $r \downarrow 0$,

$$f(r) = o(r^{1/2}),$$

$$(S_D^{-1}\Phi)(r) = \begin{pmatrix} p^+ \\ p^- \end{pmatrix} r^B + o(r^{1/2}),$$

$$r^B \Phi(r) = \begin{pmatrix} 1 \\ -\frac{1+\nu-B}{1+\nu+B} \end{pmatrix} \gamma + \begin{pmatrix} q^+ \\ q^- \end{pmatrix} r^{2B} + o(r^{1/2+B})$$

(see, respectively, (5.3.13), (5.3.12), and (5.3.8) above). Therefore, the limit in the first component yields $r^B g^+(r) \xrightarrow{r \downarrow 0} b$, and also

$$r^{-B}\big(g^+(r) - br^{-B}\big) = r^{-B}\big(f^+(r) + a(S_D^{-1}\Phi)^+(r) + b\gamma^{-1}\Phi^+(r) - br^{-B}\big)$$
$$= a\,p^+ + b\,q^+\gamma^{-1} + o(r^{1/2-B}),$$

that is, $r^{-B}(g^+(r) - br^{-B}) \xrightarrow{r \downarrow 0} a\,p^+ + b\,q^+\gamma^{-1}$. Thus, (5.3.15) and (5.3.16) follow by setting

$$g_0^+ := b, \qquad g_1^+ := ap^+ + bq^+\gamma^{-1} \tag{*}$$

(an analogous argument holds for the lower components).

(ii) Necessary and sufficient condition for $g \in \mathcal{D}(S^*)$ to belong to the domain $\mathcal{D}(S_\beta)$ of the extension S_β determined by (5.3.14) of Theorem 5.3.4 is that in the decomposition (5.3.22) above the coefficients a and b satisfy $a = \beta b\gamma^{-1}$. Owing to (*) and (5.3.18), the latter condition reads $g_1^+/g_0^+ = c_\nu\beta + d_\nu$. $\square$

Last, it is worth highlighting a couple of important remarks.

Remark 5.3.7. The proof of Theorem 5.3.5 shows that the decomposition of $g \in \mathcal{D}(S_\beta)$ determined by (5.3.14), and hence c and f, are explicitly given by

$$c = \Big(\frac{\Gamma(B)}{\Gamma(2B)} \frac{1+\nu}{1+\nu+B}\Big) \cdot \lim_{r \downarrow 0} r^B g^+(r)$$
$$f = g - c(\beta S_D^{-1}\Phi + \Phi). \tag{5.3.23}$$

Indeed, in the notation of (5.3.22) therein, $b = \gamma c$. In fact, the same argument shows that the first equation in (5.3.23) determines the component $c\Phi \in \ker S^*$ of a generic $g \in \mathcal{D}(S^*)$, and hence defines the (non-orthogonal) projection $\mathcal{D}(S^*) \to \ker S^*$, $g \mapsto c\Phi$ induced by the decomposition formula (5.3.11). When $\beta \neq 0$, one has equivalently

$$c = \beta^{-1} \int_0^{+\infty} \langle \Phi(r), (\widetilde{S}g)(r) \rangle_{\mathbb{C}^2} \, dr. \tag{5.3.24}$$

Indeed $\widetilde{S}g = S_\beta g = S^*g = \overline{S}f + c\beta\Phi$ and $\mathrm{ran}\,\overline{S} \perp \ker S^*$, whence it follows that $\langle \Phi, \widetilde{S}g \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^2)} = c\beta$.

Remark 5.3.8. As typical when the operator which one studies the self-adjoint extensions of is a differential operator, one interprets (5.3.11) as the canonical decomposition of an element $g \in \mathcal{D}(S^*)$ into a 'regular' and a 'singular' part

$$g_{\mathrm{reg}} := f + a\,S_D^{-1}\Phi \in \mathcal{D}(S_D)$$
$$g_{\mathrm{sing}} := \frac{b}{\gamma}\,\Phi \in \ker S^*, \tag{5.3.25}$$

where $a, b \in \mathbb{C}$ and $f \in \mathcal{D}(\overline{S})$ are determined by g and $\gamma = \frac{\Gamma(2B)}{\Gamma(B)} \frac{1+\nu-B}{1+\nu}$. Indeed $\mathcal{D}(S_D)$ has a higher regularity then $\ker S^*$: functions in the former space vanish at zero, as follows from (5.3.12)-(5.3.13), whereas Φ diverges at zero, as seen in (5.3.8). In this language, $r^{-B}g_{\mathrm{reg}}^+(r) \xrightarrow{r \downarrow 0} ap^+$ and $r^B g_{\mathrm{sing}}^+(r) \xrightarrow{r \downarrow 0} b$, and the self-adjointness condition (5.3.17) that selects, among the elements in $\mathcal{D}(S^*)$, only those in $\mathcal{D}(S_\beta)$ reads

$$\Big(\frac{\gamma}{p^+} \lim_{r \downarrow 0} r^{-B} g_{\mathrm{reg}}^+(r)\Big) = (c_\nu\beta + d_\nu)\Big(\lim_{r \downarrow 0} r^B g_{\mathrm{sing}}^+(r)\Big), \tag{5.3.26}$$

that is, the ratio between $\gamma(p^+)^{-1}$ times the coefficient of the leading vanishing term of g_{reg}^+ and the coefficient of the leading divergent term of g_{sing}^+ is indexed by the real extension parameter β.

5.3.1 Deficency indices

In this section we compute the deficency indices for the Dirac-Coulomb operator. As recalled in Subsection 1.3.1, given a densely defined symmetric operator T its deficency indices are

$$n_\pm := \dim \ker(T^* \mp i). \tag{5.3.27}$$

In a sense they measure 'how far' the operator T is from being self-adjoint. More precisely, by Theorem 1.3.1, a densely defined symmetric operator admits non-trivial self-adjoint extensions if and only if the deficency indices are equal and different from zero: $n_+ = n_- \neq 0$. If this is true and $n_+ < \infty$, then all the self-adjoint extensions of T are parametrized by n_+^2 real parameters.

Theorem 5.3.9 ([119], Theorem 6.9). *Let H be the Dirac operator with Coulomb potential with $V(x) = \frac{\nu}{|x|} \mathbb{1}$ defined on $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$. Then the deficency indices are*

i) $(0,0)$ *if* $|\nu| \leqslant \frac{\sqrt{3}}{2}$;

ii) $(2n(n+1), 2n(n+1))$ *if* $\sqrt{n^2 - \frac{1}{4}} < |\nu| \leqslant \sqrt{(1+n)^2 - \frac{1}{4}}$ *with* $n \in \mathbb{N}$.

Remark 5.3.10. The deficency indices for the Dirac operator with scalar potential are the same even if we relax the hypothesis of spherical symmetry of the potential. In fact, the statement of the theorem remains unchanged except for the fact that the inequalities become all strict. In order to compute the deficency indices for $\nu = \sqrt{n^2 - \frac{1}{4}}$ in the general case of non spherical symmetry one needs additional information on the potential (see [124] Theorem 4.2).

Proof. Using the Hilbert space decomposition (5.1.16), the operator decomposition (5.1.20) and Lemma 3.2.11, the computation of deficiency indices is reduced to the computation of deficiency indices for the ordinary differential operator h_{m_j, κ_j} defined in (5.1.21).

This computation is easily done with Weyl's alternative theorem (see Theorem 1.4.1): either for every $\lambda \in \mathbb{C}$ all solutions of $(h_{m_j, \kappa_j} - \lambda)u = 0$ are square integrable in $(0,1)$ (resp. in $(1, \infty)$), or for every $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there exists a unique (up to a multiplicative constant) solution u of $(h_{m_j, \kappa_j} - \lambda)u = 0$ which is square integrable in $(0,1)$ (resp. in $(1, \infty)$). Therefore, since no third option is possible, it is sufficient to check whether both the solutions of $h_{m_j, \kappa_j} u = 0$ are square integrable in $(0,1)$ and $(1, \infty)$.

To check if h_{m_j, κ_j} is in the limit-point or in the limit-circle case we consider the operator $(h_{m_j, \kappa_j} - \beta)$. The subtraction of a bounded operator does not change the computation of the deficency indices. Choosing $\lambda = 0$, the equation to be solved is $(h_{m_j, \kappa_j} - \beta)u = 0$. Its solutions are

$$u(r) \;=\; \begin{pmatrix} u^+(r) \\ u^-(r) \end{pmatrix} = \begin{pmatrix} \pm\sqrt{\kappa_j^2 - \nu^2} - \kappa_j \\ \nu \end{pmatrix} r^{\pm\sqrt{\kappa_j^2 - \nu^2}}. \tag{5.3.28}$$

From this explicit expression we see that the solution with positive exponent cannot be square integrable in $(1, \infty)$ and hence independently of the parameters κ_j and ν the operator is always in the limit point case at infinity.

The solution with positive exponent is always square integrable in $(0,1)$ while the one with negative square root is square integrable near zero if and only if

$$-2\sqrt{\kappa_j^2 - \nu^2} \leqslant -1, \tag{5.3.29}$$

which means

$$\nu^2 \leqslant \kappa_j^2 - \frac{1}{4}. \tag{5.3.30}$$

Then if ν satisfies (5.3.30), the operator is in the limit point case at both endpoints. By Theorem 1.4.3, if (5.3.30) holds the deficency indices of the operator are $(0,0)$, otherwise the deficency indices of the operator are $(1,1)$.

To compute the deficency indices of the full operator we have to count how many reduced operators are not essentially self-adjoint. Explicitly,

$$n_\pm = \sum_{j\in\mathbb{N}+\frac{1}{2}} \sum_{m_j=-j}^{j} \sum_{\kappa_j=\pm(j+\frac{1}{2})} \begin{cases} 1 & \text{if } \nu^2 > \kappa_j - \frac{1}{4} \\ 0 & \text{else} \end{cases} . \qquad (5.3.31)$$

Let n be the integer such that $n^2 - \frac{1}{4} < \nu^2 \leqslant (n+1)^2 - \frac{1}{4}$. We obtain

$$n_\pm = \sum_{j\in\mathbb{N}+\frac{1}{2}}^{n-\frac{1}{2}} \sum_{m_j=-j}^{j} 2 = 2n(n+1). \qquad (5.3.32)$$

$\square$

5.3.2   Homogeneous problem $\widetilde{S}u = 0$

In this Section we identify the dimension and the basis of the subspace $\ker S^*$, and prove Proposition 5.3.1. One has to solve the homogeneous differential equation $\widetilde{S}u = 0$, where $\widetilde{S}$ is the differential operator (5.3.3) and the function $r \mapsto u(r) = \begin{pmatrix} u^+(r) \\ u^-(r) \end{pmatrix}$ on $\mathbb{R}^+$ is the spinorial unknown. The needed ODE technique is classical and we include it concisely for completeness. Observe, however, that for the application of von Neumann's theory of self-adjoint extension one has to solve the ODE problem $\widetilde{S}u = zu$ for non-real $z \in \mathbb{C}$, say, $z = \pm\mathrm{i}$, which requires a somewhat more extended discussion – see, e.g., [114, Section 3] or [64, Sections 4-6].

Upon transforming the unknown u into φ, where

$$\varphi(r) \; := \; \tfrac{1}{2}(\mathbf{A}u)(\tfrac{r}{2})\, e^{r/2} \,, \qquad \mathbf{A} := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} , \qquad (5.3.33)$$

the differential system $\widetilde{S}u = 0$ takes the form

$$\begin{cases} (\varphi^+)' = \varphi^+ - \frac{1-\nu}{r}\,\varphi^- \\ (\varphi^-)' = -\frac{1+\nu}{r}\,\varphi^+ \,. \end{cases} \qquad (5.3.34)$$

Therefore, φ^- is a solution to

$$r(\varphi^-)'' + (1-r)(\varphi^-)' - \frac{\nu^2-1}{r}\,\varphi^- \; = \; 0 \,, \qquad (5.3.35)$$

equivalently,

$$\xi(r) \; := \; r^B\varphi^-(r) \qquad (5.3.36)$$

is a solution to

$$r\xi'' + (1-2B-r)\xi' + B\,\xi \; = \; 0 \,. \qquad (5.3.37)$$

The second order ODE (5.3.37) is the confluent hypergeometric equation [1, (13.1.1) and (13.1.11)], two linearly independent solutions of which are the confluent hypergeometric functions of first and second kind, that is, respectively, the Kummer function $M_{a,b}(r)$ [1, (13.1.2)] and the Tricomi function $U_{a,b}(r)$ [1, (13.1.3)], with $a = -B$ and $b = 1 - 2B$.

The solutions $\xi_0(r) := M_{-B,1-2B}(r)$ and $\xi_\infty(r) := U_{-B,1-2B}(r)$ to (5.3.37) determine, via (5.3.36) and the second of (5.3.34), two linearly independent solutions $\varphi_0 = \begin{pmatrix} \varphi_0^+ \\ \varphi_0^- \end{pmatrix}$ and $\varphi_\infty = \begin{pmatrix} \varphi_\infty^+ \\ \varphi_\infty^- \end{pmatrix}$ to (5.3.34). Using the properties

$$M'_{a,b}(r) = \frac{a}{b} M_{a+1,b+1}(r), \qquad U'_{a,b}(r) = -a\, U_{a+1,b+1}(r)$$

([1, (13.4.8) and (13.4.21)]), and the inverse transformation of (5.3.33), that is, $u(r) = 2\, e^{-r/2}(\mathbf{A}^{-1}\varphi)(2r)$, where $\mathbf{A}^{-1} = \mathbf{A}$, yields the following two linearly independent solutions to the original problem $\widetilde{S}u = 0$:

$$u_0(r) := \frac{1}{e^r r^B}\begin{pmatrix} \frac{1+\nu+B}{1+\nu} M_{-B,1-2B}(2r) + \frac{2rB}{(1+\nu)(1-2B)} M_{1-B,2-2B}(2r) \\ -\frac{1+\nu-B}{1+\nu} M_{-B,1-2B}(2r) + \frac{2rB}{(1+\nu)(1-2B)} M_{1-B,2-2B}(2r) \end{pmatrix}$$

$$u_\infty(r) := \frac{1}{e^r r^B}\begin{pmatrix} \frac{1+\nu+B}{1+\nu} U_{-B,1-2B}(2r) - \frac{2rB}{1+\nu} U_{1-B,2-2B}(2r) \\ -\frac{1+\nu-B}{1+\nu} U_{-B,1-2B}(2r) - \frac{2rB}{1+\nu} U_{1-B,2-2B}(2r) \end{pmatrix}$$

(5.3.38)

(in fact, an irrelevant common pre-factor 2^{-B} has been neglected). Both u_0 and u_∞ are real-valued and smooth on $\mathbb{R}^+$.

Because of the asymptotics [1, (13.1.2), (13.5.1), and (13.5.5)]

$$M_{a,b}(r) = \frac{e^r\, r^{a-b}}{\Gamma(a)}(1+O(r^{-1})) \qquad \text{as } r \to +\infty$$

$$M_{a,b}(r) = 1 + O(r) \qquad \text{as } r \downarrow 0 \quad \text{and } -b \notin \mathbb{N}$$

(5.3.39)

and [1, (13.1.2), (13.1.3), (13.5.2), (13.5.8), and (13.5.10)]

$$U_{a,b}(r) = r^{-a}(1+O(r^{-1})) \qquad\qquad\qquad \text{as } r \to +\infty$$

$$U_{a,b}(r) = \frac{\Gamma(1-b)}{\Gamma(1+a-b)} + \frac{\Gamma(b-1)}{\Gamma(a)} r^{1-b} + O(r) \qquad \begin{matrix}\text{as } r \downarrow 0 \\ \text{and } b \in (0,1)\end{matrix}$$

$$U_{a,b}(r) = \frac{\Gamma(b-1)}{\Gamma(a)} r^{-(b-1)} + O(1) \qquad\qquad \begin{matrix}\text{as } r \downarrow 0 \\ \text{and } b \in (1,2),\end{matrix}$$

(5.3.40)

one deduces that both u_0 and u_∞ are square-integrable around $r = 0$, whereas only u_∞ is square-integrable at infinity, and moreover

$$u_0(r) = \begin{pmatrix} \frac{1+\nu+B}{1+\nu} \\ -\frac{1+\nu-B}{1+\nu} \end{pmatrix} r^{-B} + O(r^{1-B}) \qquad\qquad \text{as } r \downarrow 0$$

$$u_0(r) = -\frac{2^B(1-2B)}{\Gamma(-B)(1+\nu)}\begin{pmatrix} 1 \\ 1 \end{pmatrix} r^B e^r (1 + O(r^{-1})) \qquad \text{as } r \to +\infty,$$

(5.3.41)

and

$$u_\infty(r) = \frac{\Gamma(2B)}{\Gamma(B)}\begin{pmatrix} \frac{1+\nu-B}{1+\nu} \\ -\frac{1+\nu+B}{1+\nu} \end{pmatrix} r^{-B} + \begin{pmatrix} q^+ \\ q^- \end{pmatrix} r^B + O(r^{1-B}) \quad \text{as } r \downarrow 0$$

$$u_\infty(r) = 2^B\begin{pmatrix} 1 \\ -1 \end{pmatrix} r^{-B} e^{-r}(1 + O(r^{-1})) \qquad \text{as } r \to +\infty,$$

(5.3.42)

where

$$q^\pm := \frac{4^B(-B\pm(1+\nu))\Gamma(-2B)}{(1+\nu)\Gamma(-B)}.$$

(5.3.43)

Observe that $q^\pm \neq 0$.

Therefore, there is only a *one*-dimensional space of solutions to $\widetilde{S}u = 0$ which are square integrable, and hence, owing to (5.3.4), $\ker S^*$ is one-dimensional. For convenience, let us choose as the spanning vector the function $\Phi := u_\infty$. Then (5.3.42) implies (5.3.8) and Proposition 5.3.1 is proved.

5.3.3   Distinguished extension S_D

In this Section we qualify the distinguished extension S_D of the operator S, and prove Proposition 5.3.2.

When comparing the approach based on von Neumann's theory, as developed, e.g., in [64], with the present one based on the Kreĭn-Višik-Birman theory, to solve the homogeneous problem $S^*u = 0$ (in the KVB strategy) or to solve the deficiency space problem $S^*u = \pm iu$ (in the von Neumann strategy) are two essentially analogous versions of the same step, from the ODE viewpoint. In contrast, the qualification of S_D (in view of Theorem 2.2.1, strictly speaking one only needs to qualify the action of S_D^{-1} on $\ker S^*$) is a specific step of the KVB strategy, and it boils down to solving the ODE problem $\widetilde{S}f = g$ for given g. Along this line, we adapt to our case the analysis done in [20] for homogeneous Schrödinger operators on half-line.

In order to set up the problem conveniently, let us first replace the pair (u_0, u_∞) of linearly independent solutions (5.3.38) to $\widetilde{S}u = 0$ to the new pair (v_0, v_∞) given by

$$
\begin{aligned}
v_0 &:= u_\infty - \frac{\Gamma(2B)}{\Gamma(B)}\, u_0 \\
v_\infty &:= u_\infty\,.
\end{aligned}
\tag{5.3.44}
$$

This preserves the linear independence of v_0 and v_∞ with the virtue of having two solutions with different power-law in the asymptotics as $r \downarrow 0$: from (5.3.44) and (5.3.41)-(5.3.42) we find

$$
\begin{aligned}
v_0(r) &= \begin{pmatrix} q^+ \\ q^- \end{pmatrix} r^B + O(r^{1-B}) \\
v_\infty(r) &= \frac{\Gamma(2B)}{\Gamma(B)} \begin{pmatrix} \frac{1+\nu+B}{1+\nu} \\ -\frac{1+\nu-B}{1+\nu} \end{pmatrix} r^{-B} + O(r^B)
\end{aligned}
\qquad \text{as } r \downarrow 0\,,
\tag{5.3.45}
$$

where $q^\pm$ is given by (5.3.43). At large distances, v_0 and v_∞ have exponential asymptotics as u_0 and u_∞, namely

$$
\begin{aligned}
v_0(r) &= -\frac{1}{2}\, \frac{2^B B}{(1+\nu)\cos(B\pi)} \begin{pmatrix} 1 \\ 1 \end{pmatrix} r^B e^r (1 + O(r^{-1})) \\
v_\infty(r) &= 2^B \begin{pmatrix} 1 \\ -1 \end{pmatrix} r^{-B} e^{-r} (1 + O(r^{-1}))
\end{aligned}
\qquad \text{as } r \to +\infty\,.
\tag{5.3.46}
$$

We then proceed with standard ODE arguments. With respect to the fundamental system (v_0, v_∞), the general solution to the inhomogeneous problem $\widetilde{S}f = g$ has the form

$$
f = A_0 v_0 + A_\infty v_\infty + f_{\text{part}}\,,
\tag{5.3.47}
$$

where A_0 and A_∞ run over $\mathbb{C}$ and f_{part} is a particular solution, namely, $\widetilde{S}f_{\text{part}} = g$. Let us determine it through the variation of constants [116, Section 2.4].

First we re-write $\widetilde{S}f = g$ in normal form as

$$
y' + \mathbf{V}(r)y = g\,, \qquad y := \mathbf{E}f\,,
\tag{5.3.48}
$$

where

$$
\mathbf{V}(r) := \frac{1}{r} \begin{pmatrix} -1 & \nu \\ -\nu & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathbf{E} := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.
\tag{5.3.49}
$$

We also introduce the Wronskian

$$
\mathbb{R}^+ \ni r \mapsto W_r(v_0, v_\infty) := \det \begin{pmatrix} v_0^+(r) & v_\infty^+(r) \\ v_0^-(r) & v_\infty^-(r) \end{pmatrix}.
\tag{5.3.50}
$$

This is precisely the Wronskian $W_r(\mathbf{E}v_0, \mathbf{E}v_\infty)$ of two fundamental solutions of the problem written in normal form, because $\det \mathbf{E} = 1$ and hence $W_r(\mathbf{E}v_0, \mathbf{E}v_\infty) = W_r(v_0, v_\infty)$. Moreover, since $\mathbf{V}(r)$ is

traceless for any $r \in \mathbb{R}^+$, Liouville's theorem implies that $W_r(-\mathbf{E}v_0, -\mathbf{E}v_\infty)$ is constant, and so is also $W_r(v_0, v_\infty)$. Therefore,

$$W_r(v_0, v_\infty) \;=\; \lim_{r \downarrow 0} W_r(v_0, v_\infty) \;=\; \tfrac{4^B B}{(1+\nu)\cos(B\pi)} \;=:\; W_0^\infty \,. \tag{5.3.51}$$

The limit in (5.3.51) above follows straightforwardly from the asymptotics (5.3.45) and from the expression (5.3.43) for $q^\pm$. Clearly, $W_0^\infty \neq 0$. Then a standard application of the method of variation of constants for the differential problem (5.1.21) and the further transformation $f = \mathbf{E}y$ yields eventually

$$f_{\text{part}}(r) \;=\; \int_0^{+\infty} G(r, \rho)\, g(\rho)\, \mathrm{d}\rho \,, \tag{5.3.52}$$

where

$$G(r, \rho) \;:=\; \begin{cases} \dfrac{1}{W_0^\infty} \begin{pmatrix} v_\infty^+(r)v_0^+(\rho) & v_\infty^+(r)v_0^-(\rho) \\ v_\infty^-(r)v_0^+(\rho) & v_\infty^-(r)v_0^-(\rho) \end{pmatrix} & \text{if } 0 < \rho < r \\[2em] \dfrac{1}{W_0^\infty} \begin{pmatrix} v_0^+(r)v_\infty^+(\rho) & v_0^+(r)v_\infty^-(\rho) \\ v_0^-(r)v_\infty^+(\rho) & v_0^-(r)v_\infty^-(\rho) \end{pmatrix} & \text{if } 0 < r < \rho \,. \end{cases} \tag{5.3.53}$$

Next, we observe the following.

Lemma 5.3.11. *The integral operator R_G on $L^2(\mathbb{R}^+, \mathbb{C}, \mathrm{d}r)$ with kernel $G(r, \rho)$ given by (5.3.53) is bounded and self-adjoint.*

Proof. For each $r, \rho \in \mathbb{R}^+$, $G(r, \rho)$ is the sum of the four terms

$$\begin{aligned} G^{++}(r, \rho) &:= G(r, \rho)\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho) \\ G^{+-}(r, \rho) &:= G(r, \rho)\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(0,1)}(\rho) \\ G^{-+}(r, \rho) &:= G(r, \rho)\, \mathbf{1}_{(0,1)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho) \\ G^{--}(r, \rho) &:= G(r, \rho)\, \mathbf{1}_{(0,1)}(r)\, \mathbf{1}_{(0,1)}(\rho) \,, \end{aligned} \tag{5.3.54}$$

where $\mathbf{1}_J$ denotes the characteristic function of the interval $J \subset \mathbb{R}^+$, and correspondingly R_G splits into the sum of four integral operators with kernel given by (5.3.54).

Now, for each entry of $G^{LM}(r, \rho)$, with $L, M \in \{+, -\}$, a point-wise estimate in (r, ρ) can be derived from the short and large distance asymptotics for v_0 and v_∞. For example, the entry $G_{11}^{++}(r, \rho)$ in the first row and first column of $G^{++}(r, \rho)$ is controlled as

$$\begin{aligned} |v_\infty^+(r)\, v_0^+(\rho)\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho)| &\lesssim e^{-r}\, e^{\rho} & \text{if } 0 < \rho < r \\ |v_0^+(r)\, v_\infty^+(\rho)\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho)| &\lesssim e^{r}\, e^{-\rho} & \text{if } 0 < r < \rho \,, \end{aligned}$$

because v_0 diverges exponentially and v_∞ vanishes exponentially as $r \to +\infty$, (5.3.46); thus,

$$|G_{11}^{++}(r, \rho)| \;\lesssim\; e^{-|r-\rho|} \,.$$

In fact, the asymptotics for v_0 and v_∞ are the same for both components, so we can also conclude that

$$\|G^{++}(r, \rho)\|_{M_2(\mathbb{C})} \;\lesssim\; e^{-|r-\rho|} \,,$$

where $\|\cdot\|_{M_2(\mathbb{C})}$ denotes the matrix norm. The estimate of the other kernels is perfectly analogous, and we find

$$\begin{aligned} \|G^{++}(r, \rho)\|_{M_2(\mathbb{C})} &\lesssim (r\rho)^B e^{-|r-\rho|}\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho) \\ \|G^{+-}(r, \rho)\|_{M_2(\mathbb{C})} &\lesssim r^B e^{-\rho}\, \mathbf{1}_{(1,+\infty)}(r)\, \mathbf{1}_{(0,1)}(\rho) \\ \|G^{-+}(r, \rho)\|_{M_2(\mathbb{C})} &\lesssim e^{-r}\rho^B\, \mathbf{1}_{(0,1)}(r)\, \mathbf{1}_{(1,+\infty)}(\rho) \\ \|G^{--}(r, \rho)\|_{M_2(\mathbb{C})} &\lesssim (r^B \rho^{-B} + r^{-B}\rho^B)\, \mathbf{1}_{(0,1)}(r)\, \mathbf{1}_{(0,1)}(\rho) \,. \end{aligned} \tag{5.3.55}$$

The last three estimates in (5.3.55) show at once that the kernels $G^{+-}(r,\rho)$, $G^{-+}(r,\rho)$, and $G^{--}(r,\rho)$ are in $L^2(\mathbb{R}^+ \times \mathbb{R}^+, M_2(\mathbb{C}), \mathrm{d}r\,\mathrm{d}\rho)$ and therefore the corresponding integral operators are Hilbert-Schmidt operators, hence bounded, on $L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r)$. The first estimate in (5.3.55) allows to conclude, by an obvious Schur test, that also the integral operator with kernel $G^{++}(r,\rho)$ is bounded on $L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r)$. This proves the overall boundedness of R_G.

The self-adjointness of R_G is clear from (5.3.53): the adjoint R_G^* of R_G has kernel $\overline{G(\rho,r)^T}$, but G is real-valued and $G(\rho,r) = G(r,\rho)$, thus proving that $R_G^* = R_G$. $\square$

The integral operator R_G has a relevant mapping property that is more directly read out from the following alternative representation. If $f_{\text{part}} = R_G\,g$, then

$$f_{\text{part}}(r) \;=\; \Theta_\infty^{(g)}(r)\,v_0(r) + \Theta_0^{(g)}(r)\,v_\infty(r)\,,\tag{5.3.56}$$

where

$$
\begin{aligned}
\Theta_0^{(g)}(r) &:= \frac{1}{W_0^\infty}\int_0^r \langle\,\overline{v_0(\rho)}\,,\,g(\rho)\,\rangle_{\mathbb{C}^2}\,\mathrm{d}\rho\\[4pt]
\Theta_\infty^{(g)}(r) &:= \frac{1}{W_0^\infty}\int_r^{+\infty} \langle\,\overline{v_\infty(\rho)}\,,\,g(\rho)\,\rangle_{\mathbb{C}^2}\,\mathrm{d}\rho
\end{aligned}\tag{5.3.57}
$$

and W_0^∞ is the constant computed in (5.3.51). Indeed, from (5.3.53),

$$
\begin{aligned}
f_{\text{part}}(r) \;&=\; \int_0^{+\infty} G(r,\rho)\,g(\rho)\,\mathrm{d}\rho\\[4pt]
&=\; \frac{1}{W_0^\infty}\begin{pmatrix} v_\infty^+(r)\\ v_\infty^-(r)\end{pmatrix}\int_0^r \big(v_0^+(\rho)g^+(\rho) + v_0^-(\rho)g^-(\rho)\big)\,\mathrm{d}\rho\\[4pt]
&\quad + \frac{1}{W_0^\infty}\begin{pmatrix} v_0^+(r)\\ v_0^-(r)\end{pmatrix}\int_r^{+\infty} \big(v_\infty^+(\rho)g^+(\rho) + v_\infty^-(\rho)g^-(\rho)\big)\,\mathrm{d}\rho\,,
\end{aligned}
$$

that is, (5.3.56).

Lemma 5.3.12. *For every* $g \in L^2(\mathbb{R}^+, \mathbb{C}^2)$ *one has*

$$\int_0^{+\infty} \frac{\|(R_G\,g)(r)\|_{\mathbb{C}^2}^2}{r}\,\mathrm{d}r \;<\; +\infty\,,\tag{5.3.58}$$

i.e.,

$$\operatorname{ran} R_G \;\subset\; \mathcal{D}[r^{-1}]\,.\tag{5.3.59}$$

Proof. It suffices to prove the finiteness of the integral in (5.3.58) only for $r \in (0,1)$, since $\int_1^{+\infty} r^{-1}\|(R_G\,g)(r)\|_{\mathbb{C}^2}^2\,\mathrm{d}r \leqslant \|R_G\|^2\|g\|_{L^2(\mathbb{R}^+,\mathbb{C}^+)}^2$. Let us represent $f = R_G\,g \in \operatorname{ran} R_G$ as in (5.3.56)-(5.3.57). For $r \in (0,1)$ one has

$$
\begin{aligned}
|\Theta_0^{(g)}(r)| &\leqslant |W_0^\infty|^{-1}\,\|v_0\,\mathbf{1}_{(0,r)}\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)}\,\|g\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)} \;\leqslant\; C_{g,\nu}\,r^{B+\frac{1}{2}}\\[4pt]
|\Theta_\infty^{(g)}(r)| &\leqslant |W_0^\infty|^{-1}\,\|v_\infty\,\mathbf{1}_{(r,\infty)}\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)}\,\|g\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)} \;\leqslant\; C_{g,\nu}
\end{aligned}
$$

for some constant $C_{g,\nu} > 0$ depending on g and ν only, having used the short distance asymptotics (5.3.45) for v_0 and v_∞. Combining now the above bounds again with (5.3.45) we see that on the interval $(0,1)$ the functions $r \mapsto \Theta_0^{(g)}(r)\,v_\infty(r)$ and $r \mapsto \Theta_\infty^{(g)}(r)\,v_0(r)$ are continuous and vanish when $r \to 0$, respectively, as $r^{1/2}$ and r^B, which makes the integral $\int_0^1 r^{-1}\|(R_G\,g)(r)\|_{\mathbb{C}^2}^2\,\mathrm{d}r$ finite. $\square$

Combining Lemmas 5.3.11 and 5.3.12 together, we are now in the condition to prove Proposition 5.3.2.

Proof of Proposition 5.3.2.

(i) and (ii). The integral operator R_G on $L^2(\mathbb{R}^+, \mathbb{C})$ with kernel given by (5.3.53) is bounded and self-adjoint owing to Lemma 5.3.11, and by construction satisfies $\widetilde{S} R_G g = g \ \forall g \in L^2(\mathbb{R}^+, \mathbb{C})$. Therefore, there is one self-adjoint extension $\mathscr{S}$ of $S_{\min} = \overline{S}$ such that $\mathscr{S} R_G g = g \ \forall g \in L^2(\mathbb{R}^+, \mathbb{C})$, whence, by self-adjointness, also $R_G \mathscr{S} h = h \ \forall h \in \mathcal{D}(\mathscr{S})$. Thus, $R_G = \mathscr{S}^{-1}$ for some invertible self-adjoint realisation $\mathscr{S}$ of S. Because of Lemma 5.3.12, the space $\mathcal{D}(\mathscr{S}) = \operatorname{ran} R_G$ is contained in the potential energy form domain $\mathcal{D}[r^{-1}]$: owing to Theorem 5.1.1(ii) then $\mathscr{S}$ must be the reduction to the subspace $\mathcal{H}_{\frac{1}{2},1}$ of the distinguished self-adjoint extension of the Dirac-Coulomb operator H: we shall denote it with S_D. As such, S_D is the unique self-adjoint realisation of S satisfying the property (5.3.9), it is invertible, and its kernel is precisely given by (5.3.53).

(iii) The decompositions (5.3.10) and (5.3.11) are canonical, once a self-adjoint extension of S is given with everywhere defined and bounded inverse: see, for instance, (2.1.4) and (2.1.5).

(iv) From the previous discussion, $\Phi = u_\infty = v_\infty$ and $S_D^{-1} \Phi = R_G v_\infty$. A closed expression for the latter function is given by (5.3.56) above, which now reads

$$S_D^{-1} \Phi \;=\; \Theta_\infty^{(v_\infty)}(r)\, v_0(r) + \Theta_0^{(v_\infty)}(r)\, v_\infty(r)\,.$$

From (5.3.57) and (5.3.45) we deduce

$$
\begin{aligned}
|\Theta_0^{(v_\infty)}(r)| \;&\leqslant\; |W_0^\infty|^{-1} \int_0^r \big|\langle \overline{v_0(\rho)}, v_\infty(\rho) \rangle_{\mathbb{C}^2}\big|\, \mathrm{d}\rho \\
&\lesssim\; \int_0^r (\rho^B + O(\rho^{1-B}))(\rho^{-B} + O(\rho^B))\, \mathrm{d}\rho \\
&=\; r + o(r) \quad \text{as } r \downarrow 0
\end{aligned}
$$

and

$$
\begin{aligned}
\Theta_\infty^{(v_\infty)}(r) \;&=\; \frac{1}{W_0^\infty} \int_r^{+\infty} \langle \overline{v_\infty(\rho)}, v_\infty(\rho) \rangle_{\mathbb{C}^2}\, \mathrm{d}\rho \\
&=\; \frac{1}{W_0^\infty} \|v_\infty\|_{L^2(\mathbb{R}^+, \mathbb{C}^2)}^2 (1 + o(1)) \quad \text{as } r \downarrow 0\,.
\end{aligned}
$$

Therefore, using again the short distance asymptotics (5.3.45),

$$(S_D^{-1}\Phi)(r) \;=\; \frac{\|v_\infty\|_{L^2(\mathbb{R}^+, \mathbb{C}^2)}^2}{W_0^\infty} \begin{pmatrix} q^+ \\ q^- \end{pmatrix} r^B + o(r^B) \qquad (*)$$

where $q^\pm$ is given by (5.3.43). Upon setting

$$p^\pm \;:=\; q^\pm (W_0^\infty)^{-1} \|v_\infty\|_{L^2(\mathbb{R}^+, \mathbb{C}^2)}^2 \qquad (5.3.60)$$

we then obtain the leading term of (5.3.12). The remainder is in fact smaller than $o(r^B)$. This can be seen by comparing the above asymptotics for $S_D^{-1}\Phi$ with the expansion (5.3.62) established in the next Section (which is valid because $S_D^{-1}\Phi \in \mathcal{D}(S_D) \subset \mathcal{D}(S^*)$), namely

$$S_D^{-1}\Phi \;=\; a_0^{(S_D^{-1}\Phi)} v_0 + a_\infty^{(S_D^{-1}\Phi)} v_\infty + b_\infty^{(S_D^{-1}\Phi)} v_0 + b_0^{(S_D^{-1}\Phi)} v_\infty\,.$$

For the latter, we have the asymptotics

$$
\begin{aligned}
(S_D^{-1}\Phi)(r) \;=\;& \mathbf{c}_0\, a_0^{(S_D^{-1}\Phi)} \left(r^B + O(r^{1-B})\right) + \mathbf{c}_\infty\, a_\infty^{(S_D^{-1}\Phi)} \left(r^{-B} + O(r^B)\right) \\
& + o(r^{1/2}) \quad \text{as } r \downarrow 0\,.
\end{aligned}
\qquad (**)
$$

as follows from (5.3.45) and (5.3.63) for some non-zero constants $\mathbf{c}_0, \mathbf{c}_\infty \in \mathbb{C}^2$. In order for $(*)$ and $(**)$ to be compatible, necessarily $a_\infty^{(S_D^{-1}\Phi)} = 0$. This implies that after the leading order r^B there comes a remainder $o(r^{1/2})$, thus completing the proof of (5.3.12). $\qquad \square$

5.3.4   Operator closure $\overline{S}$

This Section is devoted to the proof of Proposition 5.3.3. In fact we will prove a stronger result of characterisation of $\mathcal{D}(\overline{S})$, namely Propositions 5.3.15 and 5.3.16 below, from which Proposition 5.3.3 follows as a corollary.

Let us start with another useful representation of $\mathcal{D}(S^*)$. It is analogous to the operator-theoretic decomposition (5.3.10), but its formulation (and proof) is more in the ODE spirit.

Lemma 5.3.13. *For each $g \in \mathcal{D}(S^*)$ there exist, uniquely determined, constants $a_0^{(g)}, a_\infty^{(g)} \in \mathbb{C}$ and functions*

$$b_0^{(g)}(r) := \frac{1}{W_0^\infty} \int_0^r \langle\, \overline{v_0(\rho)}\,,\, (S^*g)(\rho)\,\rangle_{\mathbb{C}^2}\, \mathrm{d}\rho$$

$$b_\infty^{(g)}(r) := -\frac{1}{W_0^\infty} \int_0^r \langle\, \overline{v_\infty(\rho)}\,,\, (S^*g)(\rho)\,\rangle_{\mathbb{C}^2}\, \mathrm{d}\rho \tag{5.3.61}$$

on $\mathbb{R}^+$ such that

$$g = a_0^{(g)}\, v_0 + a_\infty^{(g)}\, v_\infty + b_\infty^{(g)}\, v_0 + b_0^{(g)}\, v_\infty\,, \tag{5.3.62}$$

where v_0 and v_∞ are the two linearly independent solutions (5.3.44) to the homogeneous problem $\widetilde{S}v = 0$ (recall that they are real and smooth on $\mathbb{R}^+$) and W_0^∞ is the constant computed in (5.3.51). Moreover, both $b_0^{(g)}(r)$ and $b_\infty^{(g)}(r)$ vanish as $r \downarrow 0$, and

$$b_\infty^{(g)}(r)\, v_0(r) + b_0^{(g)}(r)\, v_\infty(r) = o(r^{1/2}) \qquad as \ \ r \downarrow 0\,. \tag{5.3.63}$$

Proof. Let $h := S^*g = \widetilde{S}g$. Then, as already argued in (5.3.47) and (5.3.56)-(5.3.57), g is expressed in terms of h as

$$g = A_0\, v_0 + A_\infty\, v_\infty + \Theta_\infty^{(h)}\, v_0 + \Theta_0^{(h)}\, v_\infty \tag{*}$$

for some $A_0, A_\infty \in \mathbb{C}$ that are now uniquely identified by g. From (5.3.57) and (5.3.61) we see that

$$\Theta_\infty^{(h)}(r) = b_\infty^{(g)}(r)$$

$$\Theta_0^{(h)}(r) = -\frac{1}{W_0^\infty} \int_0^r \langle\, \overline{v_0(\rho)}\,,\, (S^*g)(\rho)\,\rangle_{\mathbb{C}^2}\, \mathrm{d}\rho$$

$$= b_0^{(g)}(r) - \frac{1}{W_0^\infty} \int_0^{+\infty} \langle\, \overline{v_0(\rho)}\,,\, (S^*g)(\rho)\,\rangle_{\mathbb{C}^2}\, \mathrm{d}\rho\,.$$

Then (*) implies (5.3.62) at once, upon setting

$$a_0^{(g)} := A_0 - \frac{1}{W_0^\infty} \int_0^{+\infty} \langle\, \overline{v_0(\rho)}\,,\, (S^*g)(\rho)\,\rangle_{\mathbb{C}^2}\, \mathrm{d}\rho$$

$$a_\infty^{(g)} := A_\infty$$

Observe that the constant added above to A_0 is finite and bounded by $|W_0^\infty|^{-1}\|v_0\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)}\|S^*g\|_{L^2(\mathbb{R}^+,\mathbb{C}^2)}$. As for the proof of (5.3.63), by means of the short distance asymptotics (5.3.45) for v_0 and v_∞ we find

$$|b_\infty^{(g)}(r)\, v_0(r)| \lesssim r^{-B} \int_0^r \rho^B \|g(\rho)\|_{\mathbb{C}^2}\, \mathrm{d}\rho \leqslant \int_0^r \|g(\rho)\|_{\mathbb{C}^2}\, \mathrm{d}\rho$$

$$\leqslant r^{1/2}\, \|g\|_{L^2([0,r],\mathbb{C}^2)} = o(r^{1/2})$$

and

$$|b_0^{(g)}(r)\, v_\infty(r)| \lesssim r^B \int_0^r \rho^{-B} \|g(\rho)\|_{\mathbb{C}^2}\, \mathrm{d}\rho \leqslant r^B \|\rho^{-B}\|_{L^2[0,r]} \|g\|_{L^2([0,r],\mathbb{C}^2)}$$

$$\lesssim r^{1/2}\, \|g\|_{L^2([0,r],\mathbb{C}^2)} = o(r^{1/2})\,,$$

and (5.3.63) then follows. □

The next preparatory step is to introduce, for later convenience, the Wronskian of any two square-integrable functions,

$$\mathbb{R}^+ \ni r \mapsto W_r(\psi, \phi) \;:=\; \det \begin{pmatrix} \psi^+(r) & \phi^+(r) \\ \psi^-(r) & \phi^-(r) \end{pmatrix}, \quad \psi, \phi \in L^2(\mathbb{R}^+, \mathbb{C}^2), \tag{5.3.64}$$

and the boundary form for any two functions in $\mathcal{D}(S^*)$,

$$\omega(g, h) \;:=\; \langle S^* g, h \rangle - \langle g, S^* h \rangle, \qquad g, h \in \mathcal{D}(S^*). \tag{5.3.65}$$

The boundary form is antisymmetric, i.e.,

$$\omega(h, g) \;=\; -\overline{\omega(h, g)}, \tag{5.3.66}$$

and it is related to the Wronskian by

$$\omega(g, h) \;=\; -\lim_{r \downarrow 0} W_r(\overline{g}, h). \tag{5.3.67}$$

Indeed, using $\widetilde{S} = \mathbf{E} \frac{\mathrm{d}}{\mathrm{d}r} + \mathbf{V}(r)$ from (5.3.48)-(5.3.49), one has

$$\begin{aligned} \omega(g, h) \;&=\; \int_0^{+\infty} \mathrm{d}r \left(\langle (\widetilde{S}g)(r), h(r) \rangle_{\mathbb{C}^2} - \langle g(r), (\widetilde{S}h)(r) \rangle_{\mathbb{C}^2} \right) \\ &=\; \int_0^{+\infty} \mathrm{d}r \left(\langle \mathbf{E}g'(r), h(r) \rangle_{\mathbb{C}^2} - \langle g(r), \mathbf{E}h'(r) \rangle_{\mathbb{C}^2} \right) \\ &=\; \lim_{r \downarrow 0} \left(\overline{g^-(r)}\, h^+(r) - \overline{g^+(r)}\, h^-(r) \right) \;=\; -\lim_{r \downarrow 0} W_r(\overline{g}, h). \end{aligned}$$

It is also convenient to introduce the (two-dimensional) space of solutions to the differential problem $\widetilde{S}v = 0$,

$$\mathcal{L} \;:=\; \{ v : \mathbb{R}^+ \to \mathbb{C}^2 \,|\, \widetilde{S}v = 0 \} \;=\; \mathrm{span}\{v_0, v_\infty\}, \tag{5.3.68}$$

As well known, $r \mapsto W_r(u, v)$ is constant whenever $u, v \in \mathcal{L}$, and this constant is zero if and only if u and v are linearly dependent. It will be important also to keep into account that any $v \in \mathcal{L}$ is square-integrable around $r = 0$, as determined in (5.3.45).

Lemma 5.3.14. *For given $v \in \mathcal{L}$,*

$$\begin{aligned} L_v : \mathcal{D}(S^*) &\to \mathbb{C} \\ g &\longmapsto L_v(g) \;:=\; \lim_{r \downarrow 0} W_r(\overline{v}, g) \end{aligned} \tag{5.3.69}$$

defines a linear functional on $\mathcal{D}(S^*)$ which vanishes on $\mathcal{D}(\overline{S})$.

Proof. The linearity of L_v is obvious, and the finiteness of $L_v(g)$ for $g \in \mathcal{D}(S^*)$ is checked as follows. Let us decompose $g = a_0^{(g)} v_0 + a_\infty^{(g)} v_\infty + b_\infty^{(g)} v_0 + b_0^{(g)} v_\infty$ as in (5.3.62) and $v = c_0 v_0 + c_\infty v_\infty$ in the basis of $\mathcal{L}$. Owing to (5.3.69), it suffices to control the finiteness of $L_{v_0}(g)$ and $L_{v_\infty}(g)$. By linearity,

$$L_{v_0}(g) \;=\; a_0^{(g)} L_{v_0}(v_0) + a_\infty^{(g)} L_{v_0}(v_\infty) + L_{v_0}(b_\infty^{(g)} v_0 + b_0^{(g)} v_\infty);$$

moreover, $L_{v_0}(v_0) = \lim_{r \downarrow 0} W_r(v_0, v_0) = 0$, $L_{v_0}(v_\infty) = W_0^\infty$, $L_{v_0}(b_\infty^{(g)} v_0) = \lim_{r \downarrow 0} W_r(v_0, b_\infty^{(g)} v_0) = \lim_{r \downarrow 0} b_\infty^{(g)}(r) W_r(v_0, v_0) = 0$, and $L_{v_0}(b_0^{(g)} v_\infty) = \lim_{r \downarrow 0} W_r(v_0, b_0^{(g)} v_\infty) = \lim_{r \downarrow 0} b_0^{(g)}(r) W_r(v_0, v_\infty) = 0$. The conclusion is $L_{v_0}(g) = a_\infty^{(g)} W_0^\infty$. Analogously, $L_{v_\infty}(g) = -a_0^{(g)} W_0^\infty$, and this establishes the

finiteness of $L_v(g)$. Let us now prove now that if $f \in \mathcal{D}(\overline{S})$, then $L_v(f) = 0$. Let $\chi \in C_0^\infty([0, +\infty))$ be such that $\chi(r) = 1$ for $r \in [0, \frac{1}{2}]$ and $\chi(r) = 0$ for $r \in [1, +\infty)$. One has that $v\chi \in \mathcal{D}(S^*)$, indeed $v\chi \in L^2(\mathbb{R}^+, \mathbb{C}^2)$ and

$$
\begin{aligned}
\widetilde{S}(v\chi) \;&=\; (\mathbf{E}\tfrac{\mathrm{d}}{\mathrm{d}r} + \mathbf{V}(r))v\chi \;=\; \chi(\mathbf{E}\tfrac{\mathrm{d}}{\mathrm{d}r} + \mathbf{V}(r))v + \mathbf{E}v\chi' \\
&=\; (\widetilde{S}v)\chi + \mathbf{E}v\chi' \;=\; \mathbf{E}v\chi' \;\in\; L^2(\mathbb{R}^+, \mathbb{C}^2)\,,
\end{aligned}
$$

where we used $\widetilde{S} = \mathbf{E}\tfrac{\mathrm{d}}{\mathrm{d}r} + \mathbf{V}(r)$ and $\widetilde{S}v = 0$. Moreover, because of the behaviour of χ around $r = 0$, the Wronskians $W_r(\overline{v\chi}, g)$ and $W_r(\overline{v}, g)$ are asymptotically equal as $r \downarrow 0$, that is, $L_{v\chi} = L_v$ As a consequence of this latter fact and of (5.3.67),

$$
\begin{aligned}
L_v(f) \;&=\; L_{v\chi}(f) \;=\; \lim_{r\downarrow 0} W_r(\overline{v\chi}, f) \;=\; -\omega(v\chi, f) \\
&=\; \langle v\chi, S^*f\rangle - \langle S^*(v\chi), f\rangle \;=\; \langle v\chi, \overline{S}f\rangle - \langle v\chi, \overline{S}f\rangle \;=\; 0\,,
\end{aligned}
$$

which completes the proof. $\square$

We come now to thefirst characterisation of the space $\mathcal{D}(\overline{S})$.

Proposition 5.3.15. *Let $f \in \mathcal{D}(S^*)$. The following conditions are equivalent:*

(i) $f \in \mathcal{D}(\overline{S})$.

(ii) $\omega(f, g) = 0$ for all $g \in \mathcal{D}(S^*)$.

(iii) $L_v(f) = 0$ for all $v \in \mathcal{L}$.

(iv) *With respect to the decomposition (5.3.62) for f, $a_0^{(f)} = a_\infty^{(f)} = 0$.*

Proof. The implication (i)$\Rightarrow$(ii) follows at once from

$$
\omega(f, g) \;=\; \langle S^*f, g\rangle - \langle f, S^*g\rangle \;=\; \langle \overline{S}f, g\rangle - \langle \overline{S}f, g\rangle \;=\; 0\,.
$$

For the converse implication (ii)$\Rightarrow$(i), we observe that

$$
0 \;=\; \omega(f, g) \;=\; \langle S^*f, g\rangle - \langle f, S^*g\rangle \qquad \forall g \in \mathcal{D}(S^*)
$$

is equivalent to $\langle S^*f, g\rangle = \langle f, S^*g\rangle \ \forall g \in \mathcal{D}(S^*)$, which implies that $f \in \mathcal{D}(S^{**}) = \mathcal{D}(\overline{S})$.

The implication (i)$\Rightarrow$(iii) is given by Lemma 5.3.14. Conversely, let us assume that $L_v(f) = 0$ for all $v \in \mathcal{L}$, and let us prove that for such f one has $\omega(f, g) = 0$ for all $g \in \mathcal{D}(S^*)$. Since we already established the equivalence (i)$\Leftrightarrow$(ii), we would then conclude that $f \in \mathcal{D}(\overline{S})$, and hence (iii)$\Rightarrow$(i). Owing to the decomposition (5.3.62) for g,

$$
\omega(f, g) \;=\; a_0^{(g)}\omega(f, v_0) + a_\infty^{(g)}\omega(f, v_\infty) + \omega(f, b_\infty^{(g)} v_0) + \omega(f, b_0^{(g)} v_\infty)\,.
$$

One has

$$
\overline{\omega(f, v_0)} \;=\; -\omega(v_0, f) \;=\; \lim_{r\downarrow 0} W_r(\overline{v_0}, f) \;=\; L_{v_0}(f) \;=\; 0\,,
$$

having used (5.3.66) in the first step, (5.3.67) in the second, (5.3.69) in the third, and the assumption $L_v(f) = 0$ for all $v \in \mathcal{L}$ in the last step. Analogously,

$$
\overline{\omega(f, v_\infty)} \;=\; -\omega(v_\infty, f) \;=\; \lim_{r\downarrow 0} W_r(\overline{v_\infty}, f) \;=\; L_{v_\infty}(f) \;=\; 0\,.
$$

Therefore, $\omega(f, v_0) = \omega(f, v_\infty) = 0$, and one is left with

$$
\begin{aligned}
\overline{\omega(f, g)} &= \overline{\omega(f, b_\infty^{(g)} v_0)} + \overline{\omega(f, b_0^{(g)} v_\infty)} = -\omega(b_\infty^{(g)} v_0, f) - \omega(b_0^{(g)} v_\infty, f) \\
&= \lim_{r \downarrow 0} \left(W_r\big(b_\infty^{(g)} v_0, f\big) + W_r\big(b_0^{(g)} v_\infty, f\big) \right) \\
&= \lim_{r \downarrow 0} \left(\overline{b_\infty^{(g)}(r)} \, W_r(\overline{v_0}, f) + \overline{b_0^{(g)}(r)} \, W_r(\overline{v_\infty}, f) \right).
\end{aligned}
$$

As $r \downarrow 0$, $W_r(\overline{v_0}, f) \to L_{v_0}(f) = 0$ and $W_r(\overline{v_\infty}, f) \to L_{v_\infty}(f) = 0$, and also (as seen in Lemma 5.3.13) $b_\infty^{(g)}(r) \to 0$ and $b_0^{(g)}(r) \to 0$, whence $\omega(f, g) = 0$. This completes the proof of the implication (iii)$\Rightarrow$(i).

Last, in order to establish the equivalence (i)$\Leftrightarrow$(iv), let us decompose f as in (5.3.62), namely,

$$
f = a_0^{(f)} v_0 + a_\infty^{(f)} v_\infty + b_\infty^{(f)} v_0 + b_0^{(f)} v_\infty,
$$

and let us compute

$$
\begin{aligned}
L_{v_0}(f) &= \lim_{r \downarrow 0} W_r(\overline{v_0}, f) = a_0^{(f)} \lim_{r \downarrow 0} W_r(\overline{v_0}, v_0) + a_\infty^{(f)} \lim_{r \downarrow 0} W_r(\overline{v_0}, v_\infty) \\
&\quad + \lim_{r \downarrow 0} b_\infty^{(f)}(r) \, W_r(\overline{v_0}, v_0) + \lim_{r \downarrow 0} b_0^{(f)}(r) \, W_r(\overline{v_0}, v_\infty) \\
&= a_\infty^{(f)} W_0^\infty.
\end{aligned}
$$

Indeed, $W_r(\overline{v_0}, v_0) = W_r(v_0, v_0) = 0$, and $W_r(\overline{v_0}, v_\infty) = W_r(v_0, v_\infty) \to W_0^\infty$, $b_\infty^{(f)}(r) \to 0$, and $b_0^{(f)}(r) \to 0$ as $r \downarrow 0$. Similarly,

$$
L_{v_\infty}(f) = -a_0^{(f)} W_0^\infty.
$$

Because of the already proved equivalence (i)$\Leftrightarrow$(iii), we then conclude that $f \in \mathcal{D}(\overline{S})$ if and only if $L_{v_0}(f) = L_{v_\infty}(f) = 0$, which from the above computation is tantamount as $a_0^{(f)} = a_\infty^{(f)} = 0$. This completes the proof. $\qquad\square$

We can see that Proposition 5.3.3 is therefore an immediate corollary of Lemma 5.3.13 and Proposition 5.3.15 above. Before presenting the proof of Proposition 5.3.3, we give the following more informative characterisation of $\mathcal{D}(\overline{S})$.

Proposition 5.3.16. *The domain of the closure can be characterise as a standard functional space:*

$$
\mathcal{D}(\overline{S}) = H_0^1(\mathbb{R}^+). \tag{5.3.70}
$$

Proof. Since $\mathcal{D}(\overline{S}) \subset \mathcal{D}(S^*)$ we know that, for every $f \in \mathcal{D}(S^*)$ there exists $\psi \in \mathcal{H}$ such that $Sf = \psi$. This means

$$
\begin{cases}
\frac{\mathrm{d}f^-}{\mathrm{d}r} = -\psi^+ + \frac{1}{r}f^- + \left(1 + \frac{\nu}{r}\right)f^+ \\
\frac{\mathrm{d}f^+}{\mathrm{d}r} = \psi^+ - \frac{1}{r}f^+ - \left(\frac{\nu}{r} - 1\right)f^-
\end{cases}
$$

From these equations one concludes that $\frac{\mathrm{d}f^+}{\mathrm{d}r}, \frac{\mathrm{d}f^-}{\mathrm{d}r} \in L^2(\mathbb{R}^+)$. Indeed $\psi^\pm \in L^2(\mathbb{R}^+)$ by hypothesis and $\frac{1}{r}f^\pm \in L^2(\mathbb{R}^+)$ because $f^\pm \in L^2(\mathbb{R}^+)$ and (5.3.63). Hence $f^\pm \in H^1(\mathbb{R}^+)$. Since $f^\pm(0) = 0$ we conclude $f^\pm \in H_0^1(\mathbb{R}^+)$, meaning that $f \in H_0^1(\mathbb{R}^+, \mathbb{C}^2)$. This proves $\mathcal{D}(\overline{S}) \subset H_0^1(\mathbb{R}^+)$.

The opposite inclusion is trivial because if $f \in H_0^1(\mathbb{R}^+, \mathbb{C}^2)$, then $f \in \mathcal{D}(S^*)$ because $Sf \in L^2(\mathbb{R}^+, \mathbb{C}^2)$ and $|f(r)| \leqslant \int_0^r |f'(\rho)| \, \mathrm{d}\rho \leqslant \|f'\|_{L^2([0,r], \mathbb{C}^2)} r^{1/2} = o(r^{1/2})$, whence $f \in \mathcal{D}(\overline{S})$ because of Proposition 5.3.15. $\qquad\square$

Proof of Proposition 5.3.3. The vanishing limit (5.3.13) for a generic $f \in \mathcal{D}(\overline{S})$ follows from the fact that, owing to Proposition 5.3.15(iv), $f = b_\infty^{(f)} v_0 + b_0^{(f)} v_\infty$, and from the asymptotics (5.3.63) of Lemma 5.3.13. The H^1-regularity of f on any interval $[\varepsilon, +\infty)$, with $\varepsilon > 0$, follows from the fact that on such interval the r^{-1} potential is bounded and hence the closure of $\mathcal{D}(S)$ in the graph norm is in fact the closure of the smooth and compactly supported functions in the H^1-norm.

Equality of function spaces follows from Proposition 5.3.16. $\hfill\square$

5.3.5   Resolvents and spectral gap

In this Section we give the details of the derivation of a couple of relevant consequences from the general classification Theorem 2.2.1, which concern the invertibility of each member of the family of self-adjoint extensions and the expression of the resolvent. As an application to the Dirac-Coulomb Hamiltonian under consideration, we then prove Theorem 5.3.6.

In fact, Theorem 5.3.17 below is standard within the Kreĭn-Višik-Birman extension theory for semi-bounded operators (see Section 2.4): we present for completeness the proof in the more general framework of self-adjoint extensions of a symmetric operator with a distinguished, invertible extension. An analogous argument, from a somewhat different perspective, can be found in [60, Theorems 13.8, 13.23, and 13.25].

Theorem 5.3.17 (Invertibility of extensions and resolvents). *Let S be a densely defined symmetric operator on a Hilbert space $\mathcal{H}$ which admits a self-adjoint extension S_D that has everywhere defined and bounded inverse on $\mathcal{H}$. In terms of the parametrisation (2.2.1) of Theorem 2.2.1, let S_T be a generic self-adjoint extension of S and $P_T : \mathcal{H} \to \mathcal{H}$ be the orthogonal projection onto $\overline{\mathcal{D}(T)}$, where the operator T is the extension parameter.*

(i) *S_T is invertible on the whole $\mathcal{H}$ if and only if T is invertible on the whole $\overline{\mathcal{D}(T)}$.*

(ii) *When S_T is invertible, and so is T, because of (i), one has*

$$S_T^{-1} = S_D^{-1} + P_T T^{-1} P_T . \tag{5.3.71}$$

(iii) *Assume further that $\dim \ker S^* = 1$, i.e., S has deficiency indices (1,1). Let $\widehat{S}$ be a self-adjoint extension of S other than the distinguished extension S_D. Let $\Phi \in \ker S^* \setminus \{0\}$ and for each $z \in \rho(\widehat{S}) \cap \mathbb{R}$ set*

$$\Phi(z) := \Phi + z(S_D - zI)^{-1}\Phi \ \in \ \ker(S^* - z\mathbb{1}) . \tag{5.3.72}$$

Then there exists an analytic function $\eta : \rho(\widehat{S}) \cap \mathbb{R} \to \mathbb{R}$ with $\eta(z) \neq 0$, such that

$$(\widehat{S} - zI)^{-1} = (S_D - zI)^{-1} + \eta(z)|\Phi(z)\rangle\langle\Phi(z)| . \tag{5.3.73}$$

$\eta(z)$, $\Phi(z)$ and (5.3.73) admit an analytic continuation to $\rho(S_D) \cap \rho(\widehat{S})$.

Proof. (i) Let us show first that S_T is injective if and only if T is injective. Assume that S_T is injective and pick $v \in \mathcal{D}(T)$ such that $Tv = 0$. Then v is an element in $\mathcal{D}(S_T)$, because it is a vector of the form (2.2.1), namely $g = f + S_D^{-1}(Tv + w) + v$, with $f = w = 0$. Since $S_T v = 0$ by injectivity one concludes that $v = 0$. Conversely if T is injective and for some $g = f + S_D^{-1}(Tv + w) + v \in \mathcal{D}(S_T)$ one has $S_T g = 0$, then $\overline{S}f + Tv + w = 0$ Since $\overline{S}f + Tv + w \in \mathrm{ran}\overline{S} \boxplus \mathrm{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$, one must have $\overline{S}f = Tv = w = 0$. Owing to the injectivity of $\overline{S}$ and T, $f = v = 0$ and hence $g = 0$. Next, let us show that S_T is surjective if and only if T is surjective. One has $\mathrm{ran}S_T = \mathrm{ran}\overline{S} \boxplus \mathrm{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp)$ and in fact $\mathrm{ran}\overline{S} = \overline{\mathrm{ran}S}$. Thus T is surjective if and only if $\mathrm{ran}T \boxplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \overline{\mathrm{ran}T} \oplus (\ker S^* \cap \mathcal{D}(T)^\perp) = \ker S^*$, if and only if $\mathrm{ran}S_T = \overline{\mathrm{ran}S} \oplus \ker S^* = \mathcal{H}$ if and only if S_T is surjective. The proof of (i) is thus completed.

(ii) (5.3.71) is an identity between bounded self-adjoint operators. For a generic $h \in \operatorname{ran} S_T$ one has $h = S_T g$ for some $g = f + S_D^{-1}(Tv + w) + v = F + v$, where $f \in \mathcal{D}(S_{min})$, $v \in \mathcal{D}(T)$, $w = \ker S^* \cap \mathcal{D}(T)$ (Theorem 2.2.1), and hence $F \in \mathcal{D}(S_D)$. Then

$$\langle h, S_T^{-1} h \rangle = \langle g, S_T g \rangle = \langle F, S_D F \rangle + \langle v, Tv \rangle.$$

On the other hand

$$\langle F, S_D F \rangle = \langle S_D F, S_D^{-1} S_D F \rangle = \langle S_T g, S_D^{-1} S_T g \rangle = \langle h, S_D^{-1} h \rangle$$

and

$$\langle v, Tv \rangle = \langle Tv, T^{-1} Tv \rangle = \langle P_T S_T g, T^{-1} P_T S_T g \rangle = \langle h, P_T T^{-1} P_T h \rangle$$

whence the conclusion $\langle h, S_T^{-1} h \rangle = \langle h, S_D^{-1} h \rangle + \langle h, P_T T^{-1} P_T h \rangle$.

(iii) Even without assuming for the moment unital deficiency indices, for $z \in \rho(\widehat{S}) \cap \rho(S_D)$ let $T(z)$ be the extension parameter, in the sense of KVB parametrisation (2.2.1) of Theorem 2.2.1, of the operator $\widehat{S} - z\mathbb{1}$ considered as a self-adjoint extension of the densely defined operator $S(z) = S - z\mathbb{1}$. Correspondingly, let $P(z)$ be the orthogonal projection onto $\overline{\mathcal{D}(T(z))}$. Then

$$(\widehat{S} - z\mathbb{1})^{-1} = (S_D - z\mathbb{1})^{-1} + P(z) \, T(z)^{-1} P(z), \tag{*}$$

which follows from part (ii), due to the fact that the distinguished extension of $S - z\mathbb{1}$ is $S_D - z\mathbb{1}$. Assuming now $\dim \ker S^* = 1$, one has $\dim \ker(S^* - z\mathbb{1}) = 1$, because of the constancy of the deficiency indices. Moreover, $\widehat{S} - z\mathbb{1}$ is a self-adjoint extension of $S - z\mathbb{1}$, whose extension parameter $T(z)$, in the sense of KVB parametrisation of Theorem 2.2.1, acts as the multiplication by a real number $t(z)$ on the one-dimensional space $\ker(S^* - z\mathbb{1})$. The fact that $(S^* - z\mathbb{1})\Phi(z) = 0$ is obvious by construction. Moreover $\Phi(z) \neq 0$ for each admissible z: this is obviously true if $z = 0$, and if it was not true for $z \neq 0$, then $z(S_D - z\mathbb{1})^{-1}\Phi = -\Phi \neq 0$, which would contradict $\mathcal{D}(S_D - z\mathbb{1}) \cap \ker(S^* - z\mathbb{1}) = \{0\}$. Thus, $\Phi(z)$ spans $\ker(S^* - z\mathbb{1})$ and $P_T := \|\Phi(z)\|^{-2} |\Phi(z)\rangle\langle\Phi(z)| : \mathcal{H} \to \mathcal{H}$ is the orthogonal projection onto $\ker(S^* - z\mathbb{1})$. In this case, the resolvent formula (*) above takes precisely the form (5.3.73) where $\eta(z) := \|\Phi(z)\|^{-2} t(z)^{-1}$. Being a product of non-zero quantities, $\eta(z) \neq 0$. Moreover, $z \mapsto (\widehat{S} - z\mathbb{1})^{-1}$ and $z \mapsto (S_D - z\mathbb{1})^{-1}$ are analytic operator-valued functions on the whole $\rho(S_D) \cap \rho(\widehat{S})$ (because of the analyticity of resolvents) and so is the vector-valued function $z \mapsto \Phi(z)$ (because of the construction (5.3.72)). Therefore, taking the expectation of both sides of (*) on $\Phi(z)$ shows at once that $z \mapsto \eta(z)$ is analytic on $\rho(S_D) \cap \rho(\widehat{S})$, and real analytic on $\mathbb{R} \cap \rho(\widehat{S})$. $\qquad\square$

Proof of Theorem 5.3.6. Part (i) is an immediate consequence of Theorem 5.3.17(i), since the KVB-extension parameter in the present case is the multiplication by β. This is of course consistent with the representation formula (5.3.14), which clearly implies that when $\beta = 0$ the extension $S_{\beta=0}$ has a kernel. Analogously, part (ii) is an immediate consequence of Theorem 5.3.17(ii), because the orthogonal projection P_T has in the present case the expression $P_T = \|\Phi\|^{-2} |\Phi\rangle\langle\Phi|$. Concerning part (iii), (5.3.20) is a consequence of the fact that, as stated in (5.3.19), the resolvent difference between the β-extension and the distinguished extension is compact. Moreover, using (5.3.19) we re-write $S_\beta f = Ef$ as

$$f = E \, S_\beta^{-1} f = E \left(S_D^{-1} + \frac{1}{\beta \|\Phi\|^2} \, |\Phi\rangle\langle\Phi| \right) f.$$

This equation is surely solved by $f = 0$ and, if $E \in (-E(\beta), E(\beta))$, then the operator acting on the r.h.s. is a contraction. Thus $f = 0$ is the only function which satisfies the eigenvalue equation $S_\beta f = Ef$ and therefore there cannot be eigenvalues in such a regime of E. $\qquad\square$

5.4   Sommerfeld's eigenvalue formula revisited and spectrum of h_D

Prior to addressing the study of the discrete spectrum of the generic self-adjoint realisation h_β (the essential spectrum being given by (5.1.8)), it is instructive to revisit the two main methods by which Sommerfeld's formula has been known since long for the eigenvalue problem of the differential operator $\widetilde{h}$ given by (5.1.21), which will be the object of this Section.

The material is undoubtedly classical, and standard references will be provided below. Our perspective here is to highlight how such standard methods for the determination of the eigenvalues of $\widetilde{h}$ actually select the discrete spectrum of the distinguished realisation h_D or of a 'mirror' distinguished one, and as such are not applicable to the other realisations of $\widetilde{h}$.

In the next Section we shall indeed discuss how Sommerfeld's formula and its actual derivation gets modified for a generic extension h_β.

For concreteness, let us assume throughout this Section that $k = 1$ and $\nu > 0$. We therefore consider the eigenvalue problem

$$h_\beta \psi \;=\; E\psi\,, \qquad \psi \in \mathcal{D}(h_\beta)\,, \qquad E \in (-1,1) \tag{5.4.1}$$

where $h = h_{m_j,k}$ given by (5.1.21), and hence the differential problem $\widetilde{h}\psi = E\psi$ with $\widetilde{h}$ being the formal expression of h.

5.4.1   The eigenvalue problem by means of truncation of asymptotic series

The historically first approach (see, e.g., [14, Section 14]) for the determination of the eigenvalues of the Dirac-Coulomb Hamiltonian is based on ODE methods.

By direct inspection it is seen that the two linearly independent solutions to $\widetilde{h}\psi = E\psi$ have large-r asymptotics $e^{r\sqrt{1-E^2}}$ and $e^{-r\sqrt{1-E^2}}$, only the second one being square-integrable and hence admissible. This suggests the natural re-scaling $\psi \mapsto U\psi =: \phi$ defined by

$$(U\psi)(\rho) \;:=\; \frac{1}{\sqrt{2}(1-E^2)^{1/4}}\,\exp\Big(\frac{\rho}{2\sqrt{1-E^2}}\Big)\,\psi\Big(\frac{\rho}{2\sqrt{1-E^2}}\Big)\,, \tag{5.4.2}$$

which induces the unitary operator $U : L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r) \to L^2(\mathbb{R}^+, \mathbb{C}^2, e^{-\rho}\,\mathrm{d}\rho)$ and yields the unitarily equivalent problem

$$U(h_\beta - E\mathbb{1})U^{-1}\phi \;=\; 0\,, \qquad \phi \;:=\; U\psi \;\in\; U\mathcal{D}(h_\beta)\,, \tag{5.4.3}$$

where

$$U(h_\beta - E\mathbb{1})U^{-1} \;=\; 2\sqrt{1-E^2}\begin{pmatrix} \frac{1}{2}\sqrt{\frac{1-E}{1+E}} + \frac{\nu}{\rho} & \frac{1}{2} - \frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{1}{\rho} \\ -\frac{1}{2} + \frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{1}{\rho} & -\frac{1}{2}\sqrt{\frac{1+E}{1-E}} + \frac{\nu}{\rho} \end{pmatrix}. \tag{5.4.4}$$

The operator (5.4.4) has a pole of order one at $\rho = 0$, implying that the differential equation (5.4.3) can be recast as

$$\rho\,\phi' \;=\; A(\rho)\,\phi \tag{5.4.5}$$

with

$$A(\rho) \;:=\; \begin{pmatrix} -1 & -\nu \\ \nu & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & \sqrt{\frac{1+E}{1-E}} \\ \sqrt{\frac{1-E}{1+E}} & 1 \end{pmatrix}\rho\,. \tag{5.4.6}$$

In particular it is explicitly checked that $\rho \mapsto A(\rho)$ is holomorphic.

It turns out that the differential problem (5.4.5)-(5.4.6) is suited for the following standard result in the theory of ordinary differential equations (see, e.g., [116, Theorems 5.1 and 5.4]).

Proposition 5.4.1. *Let $z \mapsto B(z)$ be a matrix-valued function whose entries are holomorphic at $z = 0$ and whose Taylor series $B(z) = \sum_{j=0}^{\infty} B_j z^j$, say, of radius of convergence r_B, has the zero-th component B_0 diagonal and with eigenvalues that do not differ by integers. Then there exists a holomorphic matrix-valued function $z \mapsto P(z)$ whose Taylor series $P(z) = \sum_{j=0}^{\infty} P_j z^j$ converges for $|z| < r_B$ and has zero-th component $P_0 = \mathbb{1}$, such that the transformation*

$$y(z) \; = \; P(z)f(z) \tag{5.4.7}$$

reduces the differential equation

$$zy'(z) \; = \; B(z)y(z) \tag{5.4.8}$$

to the form

$$zf'(z) \; = \; B_0 f(z). \tag{5.4.9}$$

Proposition 5.4.1 is indeed applicable to (5.4.5)-(5.4.6) whenever $\nu \in (0,1) \backslash \{ \frac{\sqrt{3}}{2} \}$ because in this case the matrix $A_0 = A(0)$ is diagonalizable and its two distinct eigenvalues $\pm B = \pm \sqrt{1 - \nu^2}$ do not differ by an integer (indeed, $2B \notin \mathbb{Z}$). (For the purpose of the discussion of this Section, we do not need to cover the exceptional case $\nu = \frac{\sqrt{3}}{2}$ which presents particular features – see, e.g., [40].)

Let us discuss first the (more relevant) critical regime $\nu \in (\frac{\sqrt{3}}{2}, 1)$: the argument for the sub-critical values $\nu \in (0, \frac{\sqrt{3}}{2})$ is even simpler and will be discussed at the end of this Subsection.

Proposition 5.4.1 implies at once that the *general solution* to (5.4.5)-(5.4.6) has the form

$$\phi(\rho) \; = \; GP(\rho) \begin{pmatrix} \rho^B & 0 \\ 0 & \rho^{-B} \end{pmatrix} \phi_0 \tag{5.4.10}$$

for some holomorphic matrix-valued $P(\rho)$ and some vector $\phi_0 \in \mathbb{C}^2$, where G is the matrix that diagonalises A_0. Component-wise,

$$\phi^+(\rho) \; = \; \sum_{j=0}^{\infty} a_j^{(B)} \rho^{B+j} + \sum_{j=0}^{\infty} a_j^{(-B)} \rho^{-B+j} \tag{5.4.11}$$

$$\phi^-(\rho) \; = \; \sum_{j=0}^{\infty} b_j^{(B)} \rho^{B+j} + \sum_{j=0}^{\infty} b_j^{(-B)} \rho^{-B+j} \tag{5.4.12}$$

for suitable coefficients $a_j^{(B)}, b_j^{(B)}, a_j^{(-B)}, b_j^{(-B)} \in \mathbb{C}$, $j \in \mathbb{N}_0$, that must satisfy the consistency relations obtained by plugging (5.4.11)-(5.4.12) into (5.4.5). In doing so, one recognises that ρ^{B+j}-powers and ρ^{-B+j}-powers never get multiplied among themselves, and moreover each type of powers only gets multiplied by a_j or b_j coefficient of the same type; the net result, when equating to zero the coefficients of each power in the identity $\rho\phi'(\rho) - A(\rho)\phi(\rho) = 0$ is the *double set* of recursive equations

$$\tfrac{1}{2} \sqrt{\tfrac{1-E}{1+E}} \, a_j^{(\pm B)} + \nu \, a_{j+1}^{(\pm B)} + \tfrac{1}{2} b_j^{(\pm B)} + (-j \mp B) b_{j+1}^{(\pm B)} \; = \; 0 \tag{5.4.13}$$

$$-\tfrac{1}{2} a_j^{(\pm B)} + (j \pm B + 2) \, a_{j+1}^{(\pm B)} - \tfrac{1}{2} \sqrt{\tfrac{1+E}{1-E}} \, b_j^{(\pm B)} + \nu \, b_{j+1}^{(\pm B)} \; = \; 0 \tag{5.4.14}$$

$$\nu \, a_0^{(\pm B)} - (\pm B - 1) b_0^{(\pm B)} \; = \; 0 \, , \tag{5.4.15}$$

that is, the upper signs for the B-part and the lower signs for the $-B$-part of (5.4.11)-(5.4.12).

The above recursive relations are conveniently re-written in a more manageable form upon introducing $\alpha_j^{(\pm B)}$ and $\beta_j^{(\pm B)}$ through

$$a_j^{(\pm B)} \; = \; \sqrt{1+E} \, (\alpha_j^{(\pm B)} + \beta_j^{(\pm B)}), \qquad b_j^{(\pm B)} \; = \; \sqrt{1-E} \, (\alpha_j^{(\pm B)} - \beta_j^{(\pm B)}), \tag{5.4.16}$$

which yields

$$\left(\tfrac{\nu}{\sqrt{1-E^2}}+1\right)\alpha_j^{(\pm B)} + \left(\tfrac{E\nu}{\sqrt{1-E^2}}+j\pm B\right)\beta_j^{(\pm B)} \quad = \quad 0 \tag{5.4.17}$$

$$\alpha_j^{(\pm B)} + \left(\tfrac{E\nu}{\sqrt{1-E^2}}-j-1\mp B\right)\alpha_{j+1}^{(\pm B)} + \left(\tfrac{\nu}{\sqrt{1-E^2}}-1\right)\beta_{j+1}^{(\pm B)} \quad = \quad 0 \tag{5.4.18}$$

$$\left(\tfrac{\nu E}{\sqrt{1-E^2}}\mp B\right)\alpha_0^{(\pm B)} - \left(\tfrac{\nu}{\sqrt{1-E^2}}-1\right)\beta_0^{(\pm B)} \quad = \quad 0\,. \tag{5.4.19}$$

Now, plugging (5.4.17) into (5.4.18) yields

$$\alpha_{j+1}^{(\pm B)} \quad = \quad \frac{\tfrac{E\nu}{\sqrt{1-E^2}}+j\pm B+1}{(j\pm B+1)^2 - B^2}\,\alpha_j^{(\pm B)}\,. \tag{5.4.20}$$

From (5.4.20) one sees that, unless $\alpha_{j_0}^{(\pm B)}=0$ for some j_0, in which case $\alpha_j^{(\pm B)}=0$ for all $j \geqslant j_0$, one has

$$\frac{\alpha_{j+1}^{(\pm B)}}{\alpha_j^{(\pm B)}} \quad = \quad j^{-1} + O(j^{-2}) \qquad \text{as } j \to +\infty\,, \tag{5.4.21}$$

implying that $\sum_j \alpha_j^{(\pm B)}\rho^j$ grows faster than $e^{\rho/2}$ at infinity and hence fails to belong to $L^2(\mathbb{R}^+,\mathbb{C},e^{-\rho}\,\mathrm{d}\rho)$. Through the transformation (5.4.16) this implies that

- at least one among $\sum_j a_j^{(B)}\rho^{B+j}$ and $\sum_j b_j^{(B)}\rho^{B+j}$,

- and at least one among $\sum_j a_j^{(-B)}\rho^{-B+j}$ and $\sum_j b_j^{(-B)}\rho^{-B+j}$

are series that diverge faster than $e^{\rho/2}$. This poses the issue of admissibility (in particular, of the square-integrability) of the spinor-valued function ϕ given by (5.4.11)-(5.4.12), for which the only possible affirmative answers are the following three.

First case: $\phi \in L^2(\mathbb{R}^+,\mathbb{C}^2,e^{-\rho}\,\mathrm{d}\rho)$ because the B-series in (5.4.11) and the B-series in (5.4.12) are actually truncated (i.e., polynomials), whereas the $(-B)$-series in (5.4.11) and the $(-B)$-series in (5.4.12) vanish identically. This is obtained by imposing that $\alpha_{n+1}^{(B)}=0$ for some $n \in \mathbb{N}_0$ and that all the $a_j^{(-B)}$'s and $b_j^{(-B)}$'s vanish. Then (5.4.20) constrains E to attain one of the values

$$E_n = -\left(1 + \frac{\nu^2}{(n+\sqrt{1-\nu^2})^2}\right)^{-\frac{1}{2}} \qquad n \in \mathbb{N}\,. \tag{5.4.22}$$

From (5.4.17) it is seen that the vanishing of α_{n+1} implies the vanishing of β_j for all $j \geqslant n+2$ while, from (5.4.18), one sees that $\beta_{n+1} \neq 0$. By direct inspection in (5.4.19) one sees that also $E_{n=0}$ given by (5.4.22) is an eigenvalue for which $\beta_0 \neq 0$ and $\alpha_0 = 0$ (it is crucial in this step that $\nu > 0$). Hence, for each value E_n, the corresponding ϕ has the form

$$\phi_n(\rho) \quad = \quad \rho^B e^{-\rho\sqrt{1-E_n^2}} \sum_{j=0}^{n+1} \begin{pmatrix} a_j^{(B)} \\ b_j^{(B)} \end{pmatrix} \rho^j\,, \tag{5.4.23}$$

and through the inverse transformation $\psi = U^{-1}\phi$ of (5.4.3) it is immediately recognised that ψ satisfies the boundary condition (5.3.17) with $\beta = \infty$. This leads to the discrete spectrum of the *distinguished* extension h_D: formula (5.4.22) is precisely the Sommerfeld's fine structure formula already introduced in (5.1.31).

Second case: $\phi \in L^2(\mathbb{R}^+,\mathbb{C}^2,e^{-\rho}\,\mathrm{d}\rho)$ because the $(-B)$-series in (5.4.11) and the $(-B)$-series in (5.4.12) are finite polynomials, whereas the B-series in (5.4.11) and the B-series in (5.4.12) vanish

identically. This is obtained by imposing that $\alpha_{n+1}^{(-B)} = 0$ for some $n \in \mathbb{N}_0$ and that all the $a_j^{(B)}$'s and $b_j^{(B)}$'s vanish. In this case (5.4.20) constrains E to attain one of the values

$$
\begin{aligned}
E_n &= -\left(1 + \frac{\nu^2}{(n - \sqrt{1 - \nu^2})^2}\right)^{-\frac{1}{2}} \qquad n \in \mathbb{N}, \\
E_0 &= B,
\end{aligned}
\tag{5.4.24}
$$

the value E_0 being obtained by direct inspection in (5.4.19) analogously to what done for the analogous point in the previous case) and for each such value, the corresponding ϕ has the form

$$
\phi_n(\rho) = \rho^{-B} e^{-\rho\sqrt{1 - E_n^2}} \sum_{j=0}^{n+1} \binom{a_j^{(-B)}}{b_j^{(-B)}} \rho^j .
\tag{5.4.25}
$$

Through the inverse transformation $\psi = U^{-1}\phi$ of (5.4.3) it is immediately recognised that ψ satisfies the boundary condition (5.3.17) with

$$
\beta = -\frac{d_\nu}{c_\nu} .
\tag{5.4.26}
$$

This is another self-adjoint realisation of the Dirac-Coulomb Hamiltonian, different from h_D, which arises in this second case, where discussion mirrored the discussion of the first case for the distinguished extension. We shall refer to this realisation as the '*mirror distinguished*' extension h_{MD}. We have thus found the discrete spectrum of h_{MD}, the eigenvalue formula (5.4.24) providing the modification of Sommerfeld's formula for this Dirac-Coulomb Hamiltonian.

It is crucial to observe at this point that the *two eigenvalue formulas* (5.4.22) *and* (5.4.24) *do not have any value in common*. As a consequence, even if combining together the truncation of the first case (in the B-series) and the truncation of the second case (in the $(-B)$-series) would produce a function ϕ that belongs to $L^2(\mathbb{R}^+, \mathbb{C}, e^{-\rho}\,\mathrm{d}\rho)$, such ϕ could not correspond to any definite value E, i.e., ϕ could not be a solution to (5.4.3).

Truncation in (5.4.11)-(5.4.12) produces admissible solutions only of the form of truncated series of B-type or truncated series of $(-B)$-type. This explains why the only remaining case is the following.

Third case: ϕ has the form (5.4.11)-(5.4.12) where *both* component ϕ^+ and ϕ^- contain two series that diverge faster than $e^{\rho/2}$ at infinity, whose sum however produces a compensation such that ϕ belongs to $L^2(\mathbb{R}^+, \mathbb{C}^2, e^{-\rho}\,\mathrm{d}\rho)$. This yields then an admissible eigenfunction $\psi = U^{-1}\phi$ with eigenvalue E. Matching the coefficients of the expansion

$$
\phi(\rho) = \rho^{-B} \binom{a_0^{(-B)}}{b_0^{(-B)}} + \rho^B \binom{a_0^{(B)}}{b_0^{(B)}} + \cdots \qquad \text{as } \rho \downarrow 0 ,
$$

through the transformation $\psi = U^{-1}\phi$, to the general boundary condition (5.3.17) indicates which domain $\mathcal{D}(h_\beta)$ the vector ψ belongs to.

Clearly, since in the third case above no truncation occurs in (5.4.11)-(5.4.12), the recursive formulas for the coefficients are now of no use and it is not possible to infer from them any closed formula for the eigenvalues of the realisation h_β, $\beta \notin \{-\frac{d_\nu}{c_\nu}, \infty\}$. In this sense, as announced at the beginning of this Section, the ODE methods discussed here only select the discrete spectrum (and a closed eigenvalue formula) for the distinguished extension h_D and for the mirror distinguished extension h_{MD}.

To conclude this Subsection, we observe that in the sub-critical regime $\nu \in (0, \frac{\sqrt{3}}{2})$, i.e., $B \in (\frac{1}{2}, 1)$, the argument that led to the general form (5.4.11)-(5.4.12) is precisely the same, but of course in this regime ρ^{-B} fails to be square-integrable near the origin, meaning that the whole $(-B)$-series in (5.4.11)-(5.4.12) must vanish identically. The only admissible solution is then that obtained with a truncation as in the first case, which leads again, as should be, to Sommerfeld's formula (5.4.22).

5.4.2   The eigenvalue problem by means of supersymmetric methods

A second, by now classical (see [109, 57, 30, 91]), approach to the determination of Sommerfeld's formula exploits the supersymmetric structure of the eigenvalue problem (5.4.1).

By means of the bounded and invertible linear transformation $A : L^2(\mathbb{R}^+, \mathbb{C}^2) \to L^2(\mathbb{R}^+, \mathbb{C}^2)$ defined by

$$A\xi \; := \; \begin{pmatrix} -(1+B) & \nu \\ \nu & -(1+B) \end{pmatrix} \begin{pmatrix} \xi^+ \\ \xi^- \end{pmatrix} \tag{5.4.27}$$

it is convenient to turn the problem (5.4.1) into the form

$$\begin{aligned} 0 \; &= \; \sigma_2 \, A^{-1} \, \sigma_2 \, (h_\beta - E\mathbb{1}) \, A \, \phi \\ &= \; \left[\begin{pmatrix} 0 & -\frac{\mathrm{d}}{\mathrm{d}r} + \frac{B}{r} + \frac{\nu E}{B} \\ \frac{\mathrm{d}}{\mathrm{d}r} + \frac{B}{r} + \frac{\nu E}{B} & 0 \end{pmatrix} - \begin{pmatrix} \frac{E}{B} - 1 & 0 \\ 0 & \frac{E}{B} + 1 \end{pmatrix} \right] \phi \, , \end{aligned} \tag{5.4.28}$$

having set

$$\phi \; := \; A^{-1}\psi \, . \tag{5.4.29}$$

Next, in terms of the differential operators

$$D^\pm \; := \; \pm\frac{\mathrm{d}}{\mathrm{d}r} + \frac{B}{r} + \frac{\nu E}{B} \tag{5.4.30}$$

acting on scalar functions, and of the differential operators

$$Q \; := \; \begin{pmatrix} \mathbb{0} & D^- \\ D^+ & \mathbb{0} \end{pmatrix} \qquad \text{and} \qquad H \; := \; Q^2 \; = \; \begin{pmatrix} D^- D^+ & \mathbb{0} \\ \mathbb{0} & D^+ D^- \end{pmatrix} \tag{5.4.31}$$

acting on spinor functions, equation (5.4.28) reads

$$Q\phi \; = \; \begin{pmatrix} \frac{E}{B} - 1 & 0 \\ 0 & \frac{E}{B} + 1 \end{pmatrix} \phi \, , \tag{5.4.32}$$

whence

$$H\phi \; = \; Q^2\phi \; = \; Q \begin{pmatrix} \frac{E}{B} - 1 & 0 \\ 0 & \frac{E}{B} + 1 \end{pmatrix} \phi \; = \; \begin{pmatrix} \frac{E}{B} + 1 & 0 \\ 0 & \frac{E}{B} - 1 \end{pmatrix} Q\phi \; = \; (\tfrac{E^2}{B^2} - 1) \, \phi \, , \tag{5.4.33}$$

equivalently,

$$\begin{aligned} D^+ D^- \phi^- \; &= \; (\tfrac{E^2}{B^2} - 1) \, \phi^- \\ D^- D^+ \phi^+ \; &= \; (\tfrac{E^2}{B^2} - 1) \, \phi^+ \, . \end{aligned} \tag{5.4.34}$$

Equation (5.4.33) or (5.4.34) is the actual *supersymmetric* form of (5.4.1). The structure is indeed the same as for the triple $(\mathscr{H}, \mathscr{P}, \mathscr{Q})$, where (see, e.g., [32, Section 6.3] and [111, Section 5.1]), for some densely defined operator D on $L^2(\mathbb{R}^+)$,

$$\mathscr{Q} \; := \; \begin{pmatrix} \mathbb{0} & D^* \\ D & \mathbb{0} \end{pmatrix}, \qquad \mathscr{P} \; := \; \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & -\mathbb{1} \end{pmatrix}, \qquad \mathscr{H} \; := \; \mathscr{Q}^2 \; = \; \begin{pmatrix} D^* D & \mathbb{0} \\ \mathbb{0} & D D^* \end{pmatrix} \tag{5.4.35}$$

are self-adjoint operators on $L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^+) \cong L^2(\mathbb{R}^+, \mathbb{C}^2)$ with the properties that $\mathscr{P}^2 = \mathbb{1}$, $\mathscr{P}\mathcal{D}(\mathscr{H}) = \mathcal{D}(\mathscr{H})$, $\mathscr{P}\mathcal{D}(\mathscr{Q}) = \mathcal{D}(\mathscr{Q})$, and $\{\mathscr{Q}, \mathscr{P}\} = \mathbb{0}$. Thus, $\mathscr{P}$ is an involution (the 'grading operator'), $\mathscr{Q}$ is a 'supercharge' with respect to such involution, and $\mathscr{H}$ is a Hamiltonian 'with supersymmetry'. Moreover, standard spectral arguments show that the two spectra $\sigma(D^* D)$ and $\sigma(D D^*)$ with respect to $L^2(\mathbb{R}^+)$ lie both in $[0, +\infty)$ and coincide, and in particular the eigenvalues are the same, but for possibly the value zero.

In the present case we did not elaborate on the domain of $D^\pm$ when applied to $L^2(\mathbb{R}^+)$, however it is clear that the two operators are formally adjoint to each other. The fact that the eigenvalues of $D^+ D^-$ and $D^- D^+$ relative to square-integrable eigenfunctions are non-negative follows from a trivial integration by parts; the fact that those such eigenvalues that are strictly positive are the same for both $D^+ D^-$ and $D^- D^+$ is also an immediate algebraic consequence, for $D^- D^+ f = \lambda f$ for $\lambda \neq 0$ implies that $D^+ f \neq 0$ and $D^+ D^- (D^+ f) = \lambda (D^+ f)$, the same then holding also when roles of D^+ and D^- are exchanged.

The solutions (E, ψ) to the problem (5.4.1), with chosen realisation h_β, can be read out from (5.4.33)-(5.4.34). Let us start with the 'ground state' solutions, where 'ground state' here is referred to the lowest possible eigenvalue of H, namely the value zero, and hence, because of (5.4.33), the smallest possible $|E|$ for the eigenvalue E of the considered realisation h_β. First of all, the ground state energy E_0 must satisfy $E_0^2 = B^2$, as follows from (5.4.33).

Out of the two possibilities, one is then to take $D^- \phi^- = 0$ in (5.4.34), with $E = E_0$ to be determined, which is an ODE whose solutions are the multiples of

$$\phi^-(r) = r^B e^{\frac{\nu E_0}{B} r}.$$

For such ϕ^- to be square-integrable, $\nu E_0 < 0$, thus $E_0 = -B$ since $\nu > 0$. Correspondingly, the second equation in (5.4.34) is $D^- D^+ \phi^+ = 0$ for some $\phi^+ \in L^2(\mathbb{R}^+)$. This is equivalent to $D^+ \phi^+ = 0$, thanks to the fact that D^- is the formal adjoint of D^+. The latter ODE is solved by the multiples of $r^{-B} e^{-\frac{\nu E_0}{B} r}$, which is not square-integrable at infinity, whence $\phi^+ = 0$. Alternatively, one may argue that the corresponding ϕ^+ to the above ϕ^- is read out directly from (5.4.32): it must be (a multiple of)

$$(\tfrac{E_0}{B} - 1)^{-1}(D^- \phi^-)(r) = (\tfrac{E_0}{B} - 1)^{-1}(\tfrac{d}{dr} + \tfrac{B}{r} + \tfrac{\nu E_0}{B})(r^B e^{\frac{\nu E_0}{B} r})$$

and it must be square-integrable, which forces ϕ^+ to be necessarily null, for the above function fails to be square-integrable at the origin.

We have thus found a solution (E, ϕ) to the problem (5.4.34) with smallest possible $|E|$ and square-integrable ϕ, namely the pair (E_0, ϕ_0) (up to multiples of ϕ_0) given by

$$E_0 = -B, \qquad \phi_0(r) = r^B e^{\frac{\nu E_0}{B} r} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{5.4.36}$$

Through (5.3.5) and the transformation (5.4.29), and in view of the classification (5.3.18), Theorem 5.3.5(i)-(ii), we see that (5.4.36) corresponds to the pair (E_0, ψ_0) given by

$$E_0 = -\left(1 + \frac{\nu^2}{1 - \nu^2}\right)^{-\frac{1}{2}}, \qquad \psi_0(r) = r^B e^{\frac{\nu E_0}{B} r} \begin{pmatrix} \nu \\ -(1 + B) \end{pmatrix} \in \mathcal{D}(h_D), \tag{5.4.37}$$

which is the ground state solution to the initial eigenvalue problem (5.4.1) for $\beta = \infty$, and hence for the *distinguished* self-adjoint realisation of the Dirac-Coulomb Hamiltonian.

By a completely analogous reasoning, the other possibility is to look for ground state solutions to (5.4.34) with $D^+ \phi^+ = 0$, and $E = E_0$ to be determined, an ODE solved by the multiples of

$$\phi^+(r) = r^{-B} e^{-\frac{\nu E_0}{B} r},$$

and such ϕ^+ is only square-integrable if $E_0 = B > 0$. Correspondingly, the first equation in (5.4.34) is $D^+ D^- \phi^- = 0$, equivalently, $D^- \phi^- = 0$, which is solved by multiples of $r^B e^{\frac{\nu E_0}{B} r}$; the latter function failing to be square integrable at infinity, one thus ends up with the solution (E_0, ϕ_0) (up to multiples of ϕ_0) given by

$$E_0 = B, \qquad \phi_0(r) = r^{-B} e^{-\frac{\nu E_0}{B} r} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{5.4.38}$$

Thus, again using (5.4.29), and comparing the expansion

$$r^{-B}e^{-\frac{\nu E_0}{B}r} = r^{-B} - \tfrac{\nu E_0}{B}r^{1-B} + o(r^{1-B}) \qquad \text{as } r \downarrow 0$$

with the general classification (5.3.18), whence now $g_0^+ = 1$, $g_1^+ = 0$, $c_\nu\beta + d_\nu = 0$, we see that another ground state solution to (5.4.1) is the pair (E_0, ψ_0) given by

$$E_0 = \Big(1 + \frac{\nu^2}{1-\nu^2}\Big)^{-\frac{1}{2}}, \qquad \psi_0(r) = r^{-B}e^{-\frac{\nu E_0}{B}r}\begin{pmatrix}-(1+B)\\\nu\end{pmatrix} \in \mathcal{D}(h_{MD}), \qquad (5.4.39)$$

and this is the ground state solution for the *mirror distinguished* $(\beta = -d_\nu/c_\nu)$ self-adjoint realisation h_{MD} already introduced in Subsection 5.4.1, formula (5.4.26).

Significantly, no other realisations can be monitored through the supersymmetric scheme above, but those with $\beta = \infty$ or $\beta = -d_\nu/c_\nu$.

The excited states too are determined within the supersymmetric scheme. Let

$$D_n^\pm := \pm\frac{\mathrm{d}}{\mathrm{d}r} + \frac{B_n}{r} + \frac{\nu E}{B_n}, \qquad B_n := B + n, \qquad n \in \mathbb{N}_0. \qquad (5.4.40)$$

Clearly $B = B_0$, $D^\pm = D_0^\pm$. D_n^+ and D_n^- are formally adjoint. From

$$D_n^\pm D_n^\mp = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{B_n(B_n \mp 1)}{r^2} + \frac{2\nu E}{r} + \frac{\nu^2 E^2}{B_n^2}$$

one deduces

$$D_n^\pm D_n^\mp f = \big(E^2(1 + \tfrac{\nu^2}{B_n^2}) - 1\big)f \qquad \Leftrightarrow \qquad -f'' + \tfrac{B_n(B_n\mp 1)}{r^2}f + \tfrac{2\nu E}{r}f - E^2 f = 0. \qquad (5.4.41)$$

Thus, the equation in (5.4.41) with the lower signs is the same as the equation with the upper signs and with B_n replaced by B_{n+1}. This is the basis for an iterative argument, as follows.

As a first step, as a consequence of (5.4.41), the equation $D^- D^+ \phi^+ = (\frac{E^2}{B^2} - 1)\phi^+$ of the problem (5.4.33) is equivalent to $D_1^+ D_1^- \phi^+ = (E^2(1 + \frac{\nu^2}{(B+1)^2}) - 1)\phi^+$, which can be regarded as the first scalar equation of

$$\begin{pmatrix} D_1^- D_1^+ & \mathbb{0} \\ \mathbb{0} & D_1^+ D_1^- \end{pmatrix}\begin{pmatrix}\xi_1^+\\\xi_1^-\end{pmatrix} = \big(E^2(1 + \tfrac{\nu^2}{(B+1)^2}) - 1\big)\begin{pmatrix}\xi_1^+\\\xi_1^-\end{pmatrix}, \qquad \xi_1^- := \phi^+. \qquad (5.4.42)$$

The ground state solution $(E_1, \xi_1^{(\mathrm{gs})})$ to the new supersymmetric problem (5.4.42) is obtained in complete analogy to the argument that led to (5.4.36), whence

$$E_1 = -\big(1 + \tfrac{\nu^2}{(B+1)^2}\big)^{-\frac{1}{2}}, \qquad \xi_1^{(\mathrm{gs})}(r) = r^{B+1}e^{\frac{\nu E_1}{B+1}r}\begin{pmatrix}0\\1\end{pmatrix}. \qquad (5.4.43)$$

(The other solution that one would find in complete analogy to the argument that led to (5.4.38) is not square integrable.) In turn, using $\phi^+ = \xi_1^-$, (5.4.43) corresponds to a solution ϕ_1^+ to the equation $D^- D^+ \phi^+ = (\frac{E_1^2}{B^2} - 1)\phi^+$, and hence to a solution (E_1, ϕ_1) to the original problem (5.4.32)-(5.4.33), given by

$$\begin{aligned} E_1 &= -\big(1 + \tfrac{\nu^2}{(B+1)^2}\big)^{-\frac{1}{2}} < E_0 < 0 \\ \phi_1^+(r) &= r^{B+1}e^{\frac{\nu E_1}{B+1}r} \\ \phi_1^-(r) &= (\tfrac{E_1}{B} + 1)^{-1}(D^+\phi_1^+)(r). \end{aligned} \qquad (5.4.44)$$

Clearly $(D^+\phi_1^+)(r) \sim r^B$ as $r \downarrow 0$, and all together $\psi_1 := A\phi_1 \in \mathcal{D}(h_D)$: thus, (E_1, ψ_1) gives the first excited state for the eigenvalue problem (5.4.1) for the *distinguished* realisation h_D.

The procedure is repeated for the iterated supersymmetric problems

$$\begin{pmatrix} \mathbb{O} & D_{n-1}^- \\ D_{n+1}^+ & \mathbb{O} \end{pmatrix} \begin{pmatrix} \xi_{n-1}^+ \\ \xi_{n-1}^- \end{pmatrix} = \begin{pmatrix} E\sqrt{1+\frac{\nu^2}{B_{n-1}^2}} - 1 & \mathbb{O} \\ \mathbb{O} & E\sqrt{1+\frac{\nu^2}{B_{n-1}^2}} + 1 \end{pmatrix} \begin{pmatrix} \xi_{n-1}^+ \\ \xi_{n-1}^- \end{pmatrix},$$

$$\begin{pmatrix} D_n^- D_n^+ & \mathbb{O} \\ \mathbb{O} & D_n^+ D_n^- \end{pmatrix} \begin{pmatrix} \xi_n^+ \\ \xi_n^- \end{pmatrix} = \big(E^2(1+\tfrac{\nu^2}{B_n^2}) - 1\big) \begin{pmatrix} \xi_n^+ \\ \xi_n^- \end{pmatrix}, \qquad \xi_n^- = \xi_{n-1}^+. \tag{5.4.45}$$

The admissible ground state solution $(E_n, \xi_n^{(\mathrm{gs})})$ for the second equation in (5.4.45) is

$$E_n = -\big(1 + \tfrac{\nu^2}{(B+n)^2}\big)^{-\frac{1}{2}}, \qquad \xi_n^{(\mathrm{gs})}(r) = r^{B+n} e^{\frac{\nu E_n}{B+n} r} \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \tag{5.4.46}$$

then, by the first equation in (5.4.45) and the preceding iterations, the pair (E_n, ϕ_n) with

$$\phi_n := \begin{pmatrix} D_{n-1}^+ \big(r^{B+n} e^{\frac{\nu E_n}{B+n} r}\big) \\ D_0^+ D_1^+ \cdots D_{n-1}^+ \big(r^{B+n} e^{\frac{\nu E_n}{B+n} r}\big) \end{pmatrix} \tag{5.4.47}$$

gives the n-th excited state solution to the original problem (5.4.32)-(5.4.33). One immediately recognises that $\phi_n^\pm(r) \sim r^B$ as $r \downarrow 0$, whence $\psi_n := A\phi_n \in \mathcal{D}(h_D)$: thus, (E_n, ψ_n) gives the n-th excited state for the eigenvalue problem (5.4.1) for the *distinguished* realisation h_D.

With the analysis above one reproduces all energy levels of Sommerfeld's formula

$$E_n = -\big(1 + \tfrac{\nu^2}{(n+\sqrt{1-\nu^2})^2}\big)^{-\frac{1}{2}}, \qquad n \in \mathbb{N}_0 \tag{5.4.48}$$

and recognises that they all correspond to bound states for the distinguished realisation h_D of the Dirac-Coulomb Hamiltonian.

By a completely symmetric iterative analysis which starts using

$$B_n := B - n, \qquad n \in \mathbb{N}_0 \tag{5.4.49}$$

instead of (5.4.40) and the same definitions for $D_n^\pm$ one sees that also the pairs (E_n, ψ_n), with $\psi_n := A\phi_n$ and

$$E_n := -\big(1 + \tfrac{\nu^2}{(n+\sqrt{1-\nu^2})^2}\big)^{-\frac{1}{2}}, \qquad \phi_n := \begin{pmatrix} D_0^+ D_1^+ \cdots D_{n-1}^+ \big(r^{-B+n} e^{\frac{\nu E_n}{-B+n} r}\big) \\ D_{n-1}^+ \big(r^{-B+n} e^{\frac{\nu E_n}{-B+n} r}\big) \end{pmatrix}, \tag{5.4.50}$$

provide a complete set of solutions to the eigenvalue problem (5.4.1) for the *mirror distinguished* realisation h_{MD} $(\psi_n \in \mathcal{D}(h_\beta)$ for $\beta = -d_\nu/c_\nu)$.

5.5 Discrete spectrum of the generic extension

In this Section we prove Theorem 5.1.4 and Corollary 5.1.5.

For Theorem 5.1.4 we study the eigenvalue problem for h_β in the form of the differential equation (5.4.3)-(5.4.4) already identified in Subsection 5.4.1. The key point is the intimate relation between the differential operator (5.4.4) and the confluent hypergeometric equation. Exploiting such a relation yields, in the operator-theoretic language of Theorem 5.3.5, the explicit expression for the eigenfunctions of the adjoint h^* of h. Imposing further that such eigenfunctions satisfy the typical boundary condition for the h_β-extension brings eventually to the implicit eigenvalue formula (5.1.29).

Proof of Theorem 5.1.4. Let us start from the differential problem (5.4.1), re-written in the form (5.4.3)-(5.4.4).

For a solution ϕ to (5.4.3) with given $E \in (-1, 1)$ we introduce, in analogy to (5.4.16), the two scalar functions u_1 and u_2 such that

$$
\begin{aligned}
\phi^+ &= \sqrt{1+E}\,(u_1 + u_2) \\
\phi^- &= \sqrt{1-E}\,(u_1 - u_2)\,.
\end{aligned}
\tag{5.5.1}
$$

Plugging (5.5.1) into (5.4.3)-(5.4.4) yields

$$
\begin{aligned}
u_2' + \Big(\tfrac{k}{\rho} + \tfrac{\nu}{\rho\sqrt{1-E^2}}\Big)u_1 + \tfrac{\nu E}{\rho\sqrt{1-E^2}}\,u_2 &= 0 \\
-u_1' + \Big(1 + \tfrac{\nu E}{\rho\sqrt{1-E^2}}\Big)u_1 + \Big(\tfrac{\nu}{\rho\sqrt{1-E^2}} - \tfrac{k}{\rho}\Big)u_2 &= 0\,,
\end{aligned}
\tag{5.5.2}
$$

and solving for u_1 in the first equation above and plugging it into the second equation gives a second order differential equation for u_2 which, re-written for the scalar function $v := \rho^B u_2$, takes the form

$$
\rho\,v'' + (1 - 2B - \rho)\,v' - \Big(\frac{\nu E}{\sqrt{1-E^2}} - B\Big)v = 0\,.
\tag{5.5.3}
$$

Equation (5.5.3) is a confluent hypergeometric equation – we refer, e.g., to [1, Chapter 13] for its definition and for the properties that we are going to use here below. Out of the two linearly independent solutions to (5.5.3), the Kummer function $M_{a,b}(\rho)$ and the Tricomi function $U_{a,b}(\rho)$ with parameters

$$
a = \frac{\nu E}{\sqrt{1-E^2}} - B\,, \qquad b = 1 - 2B\,,
\tag{5.5.4}
$$

only the latter belongs to $L^2(\mathbb{R}^+, \mathbb{C}, e^{-\rho}\mathrm{d}\rho)$, for

$$
\begin{aligned}
M_{a,b}(\rho) &= e^r\,\tfrac{r^{a-b}}{\Gamma(a)}(1 + O(r^{-1})) \\
U_{a,b}(\rho) &= r^{-a}(1 + O(r^{-1}))
\end{aligned}
\qquad \text{as } r \to +\infty\,.
$$

With $u_2 = \rho^{-B}v = \rho^{-B}U_{a,b}(\rho)$, and with u_1 determined by (5.5.2) and the property

$$
U_{a,b}'(\rho) = -a\,U_{a+1,b+1}(\rho)\,,
$$

we reconstruct the solution ϕ by means of (5.5.1) and we find

$$
\phi^\pm(\rho) = \frac{\rho^{-B}}{k + \frac{\nu}{\sqrt{1-E^2}}}\Big(\big(B \pm \nu\sqrt{\tfrac{1-E}{1+E}} \pm k\big)U_{a,b}(\rho) + a\,\rho\,U_{a+1,b+1}(\rho)\Big)\,.
\tag{5.5.5}
$$

Correspondingly, the solution $\psi = U^{-1}\phi$ to the differential problem $\widetilde{h}\psi = E\psi$, where $U : L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r) \to L^2(\mathbb{R}^+, \mathbb{C}^2, e^{-\rho}\mathrm{d}\rho)$ is the unitary map (5.4.2), takes the form

$$
\begin{aligned}
\psi^\pm(r) = \frac{(2r\sqrt{1-E^2})^{-B}\,e^{-r\sqrt{1-E^2}}}{k + \frac{\nu}{\sqrt{1-E^2}}}\Big(&\sqrt{1 \pm E}\,\big(B \pm \nu\sqrt{\tfrac{1-E}{1+E}} \pm k\big)U_{a,b}(2r\sqrt{1-E^2}) \\
&+ 2ar\sqrt{1-E^2}\,U_{a+1,b+1}(2r\sqrt{1-E^2})\Big)\,.
\end{aligned}
\tag{5.5.6}
$$

From the above expression we deduce the asymptotics

$$
\begin{aligned}
\psi^+(r) = \ &\tfrac{\Gamma(1-b)}{\Gamma(1+a-b)}\big(B + \nu\sqrt{\tfrac{1-E}{1+E}} + k\big)r^{-B} + \tfrac{\Gamma(b-1)}{\Gamma(a)}(2\sqrt{1-E^2})^{2B}\big(\nu\sqrt{\tfrac{1-E}{1+E}} + k - B\big)r^B \\
&+ o(r^{1/2}) \qquad \text{as } r \downarrow 0\,.
\end{aligned}
\tag{5.5.7}
$$

Since $\widetilde{h}\psi = E\psi \in L^2(\mathbb{R}^+, \mathbb{C}^2, \mathrm{d}r)$, then $\psi \in \mathcal{D}(h^*)$. Therefore, comparing (5.5.4) and (5.5.7) above with the general formulas (5.3.16)-(5.3.15) of Theorem 5.3.5, we read out the coefficients

$$
\begin{aligned}
g_0^+ &= \frac{\Gamma(2B)}{\Gamma(\frac{\nu E}{\sqrt{1-E^2}}+B)}\left(\nu\sqrt{\tfrac{1-E}{1+E}} + k + B\right) \\
g_1^+ &= (2\sqrt{1-E^2})^{2B}\,\frac{\Gamma(-2B)}{\Gamma(\frac{\nu E}{\sqrt{1-E^2}}-B)}\left(\nu\sqrt{\tfrac{1-E}{1+E}} + k - B\right)
\end{aligned}
\tag{5.5.8}
$$

of the small-r expansion $\psi(r) = g_0 r^{-B} + g_1 r^B + o(r^{1/2})$.

We are now in the condition to apply our classification formula (5.3.17) to such ψ. Upon setting

$$
\mathfrak{F}_{\nu,k}(E) := \frac{g_1^+}{g_0^+} = (2\sqrt{1-E^2})^{2B}\,\frac{\Gamma(-2B)}{\Gamma(2B)}\,\frac{\Gamma(\frac{\nu E}{\sqrt{1-E^2}}+B)}{\Gamma(\frac{\nu E}{\sqrt{1-E^2}}-B)}\,\frac{\nu\sqrt{\tfrac{1-E}{1+E}}+k-B}{\nu\sqrt{\tfrac{1-E}{1+E}}+k+B}
\tag{5.5.9}
$$

we deduce from (5.5.8) and (5.3.17) that the function $\psi \in \mathcal{D}(h^*)$ determined so far actually belongs to $\mathcal{D}(h_\beta)$, and therefore is a solution to $h_\beta \psi = E\psi$, if and only if E satisfies

$$
\mathfrak{F}_{\nu,k}(E) = c_{\nu,k}\,\beta + d_{\nu,k}\,,
\tag{5.5.10}
$$

which then proves (5.1.29).

It is straightforward to deduce from the properties of the Γ-function that the map $(-1,1) \ni E \mapsto \mathfrak{F}_{\nu,k}(E)$ has the following features. $\mathfrak{F}_{\nu,k}$ has vertical asymptotes corresponding to the roots of

$$
\frac{\Gamma\left(\frac{\nu E}{\sqrt{1-E^2}}+B\right)}{\Gamma\left(\frac{\nu E}{\sqrt{1-E^2}}-B\right)} \times \frac{\nu\sqrt{\tfrac{1-E}{1+E}}+k-B}{\nu\sqrt{\tfrac{1-E}{1+E}}+k+B} = \infty\,.
\tag{5.5.11}
$$

As we shall determine in detail working out equation (5.5.11) in the proof of Corollary 5.1.5, such roots are indeed countably many and the corresponding asymptotes are located at the points $E = E_n$, with E_n given by formula (5.1.31). Therefore the asymptotes accumulate at $E = -1$ for $\nu > 0$ and at $E = 1$ for $\nu < 0$. When $\nu > 0$, in each interval (E_{n+1}, E_n), as well as in the interval $(E_{n_0}, 1)$, $\mathfrak{F}_{\nu,k}$ is smooth and strictly monotone decreasing; the value $\mathfrak{F}_\nu(1)$ is finite and negative. When $\nu < 0$ one has conversely that in each interval (E_n, E_{n+1}), as well as in the interval $(-1, E_{n_0})$, $\mathfrak{F}_{\nu,k}$ is smooth and strictly monotone increasing.

Thus, the range of $\mathfrak{F}_{\nu,k}$ is the whole real line, which makes the equation (5.5.10) always solvable for any β, again with a countable collection of roots. This completes the proof. $\qquad\square$

The behaviour of $E \mapsto \mathfrak{F}_{\nu,k}(E)$ discussed above is illustrated in Figure 5.3 for $k = 1$ and $\nu > 0$. Observe that in this case the points E_n where the vertical asymptotes are located at are all negative and $E_n \to -1$ as $n \to +\infty$. For $\beta \in (-\infty, \mathfrak{F}_{\nu,k}(1)) \cup (d_{\nu,k}, +\infty)$ all such roots are strictly negative, whereas for $\beta \in (\mathfrak{F}_{\nu,k}(1), d_{\nu,k})$ the lowest root (and only that one) is strictly positive. As to be expected, $\mathfrak{F}_{\nu,k}(0) = d_{\nu,k}$, as one can easily see by comparing the value $\mathfrak{F}_{\nu,k}(0)$ obtained from (5.5.9) with the quantity d_ν given by (5.3.43)/(5.3.18).

Let us now move to the derivation of Sommerfeld's formula from our general eigenvalue equation.

Proof of Corollary 5.1.5. The goal is to determine the roots of $\mathfrak{F}_{\nu,k}(E) = \infty$, equivalently, the roots of equation (5.5.11). For each of the four factors

$$
\begin{aligned}
P_\nu(E) &:= \Gamma\left(\tfrac{\nu E}{\sqrt{1-E^2}}+B\right) \\
Q_{\nu,k}(E) &:= \nu\sqrt{\tfrac{1-E}{1+E}} + k - B \\
R_{\nu,k}(E) &:= \nu\sqrt{\tfrac{1-E}{1+E}} + k + B \\
S_\nu(E) &:= \Gamma\left(\tfrac{\nu E}{\sqrt{1-E^2}}-B\right)
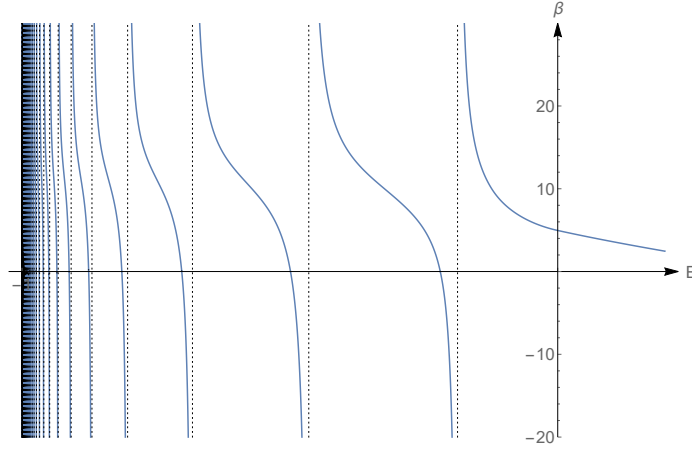\end{aligned}
$$

Figure 5.3: Plot of $\mathfrak{F}_{\nu,k}(E)$ for $k = 1$ and $\nu = 0.9$ for $E \in (-1, 0.3)$.

in the l.h.s. of (5.5.11) it is straightforward to find the following.

- $P_\nu(E) = \infty$ for $\frac{\nu E}{\sqrt{1-E^2}} + B = -n$, $n \in \mathbb{N}_0$, and hence for $E = -\mathrm{sign}(\nu)\,\mathcal{E}_n$ with

$$\mathcal{E}_n := \left(1 + \frac{\nu^2}{(n + \sqrt{1-\nu^2})^2}\right)^{-\frac{1}{2}}. \tag{5.5.12}$$

- $Q_{\nu,k}(E) = 0$ for

$$
\begin{array}{ll}
E = -B & \text{if } k = -1, \text{ and } \nu > 0 \\
E = B & \text{if } k = 1 \text{ and } \nu < 0 \\
\text{no value of } E & \text{otherwise}.
\end{array}
$$

- $R_{\nu,k}(E) = 0$ for

$$
\begin{array}{ll}
E = -B & \text{if } k = 1 \text{ and } \nu < 0 \\
E = B & \text{if } k = -1, \text{ and } \nu > 0 \\
\text{no value of } E & \text{otherwise}.
\end{array}
$$

- $S_\nu(E) = \infty$ for $\frac{\nu E}{\sqrt{1-E^2}} - B = -n$, $n \in \mathbb{N}_0$, and hence for $E = \mathrm{sign}(\nu)\,\mathcal{E}_{-n}$ with $\mathcal{E}_n$ defined in (5.5.12).

Therefore, for the problem $\mathfrak{F}_{\nu,k}(E) = \infty$, which is equivalent to

$$Z_{\nu,k}(E) := \frac{P_\nu(E)}{S_\nu(E)}\frac{Q_{\nu,k}(E)}{R_{\nu,k}(E)} = \infty,$$

we can distinguish the following cases.

For all k and ν, then $Z_{\nu,k}(E) = \infty$ at least for $E = -\mathrm{sign}(\nu)\mathcal{E}_n$ with $n \geqslant 1$ (which makes P_ν diverge, keeping $Q_{\nu,k}$, $R_{\nu,k}$, and S_ν finite); the remaining possibilities $E = \pm B$ have to be discussed separately.

If k and ν have the same sign, then $\lim_{E \to \pm B} Z_{\nu,k}(E)$ is either zero or infinity because only one among P_ν and S_ν diverges, $Q_{\nu,k}$ and $R_{\nu,k}$ remaining finite. Explicitly,

$$\lim_{E \to \mp B} Z_{\nu,k}(E) = \infty \qquad \text{if } \nu \gtrless 0$$

$$\lim_{E \to \pm B} Z_{\nu,k}(E) = 0 \qquad \text{if } \nu \gtrless 0.$$

Thus, the value $E = -\text{sgn}(\nu)B$ is admissible and $E = \text{sgn}(\nu)B$ is to be discarded. This proves formula (5.1.31) for the case k and ν with the same sign.

If instead k and ν have opposite sign, then $\lim_{E \to \pm B} Z_{\nu,k}(E)$ must be either determined resolving the indeterminate $P_\nu \cdot Q_{\nu,k} = \infty \cdot 0$ ($R_{\nu,k}$ and S_ν being finite) or resolving the indeterminate form $S_\nu \cdot R_{\nu,k} = \infty \cdot 0$ (P_ν and $Q_{\nu,k}$ being finite). Owing to the asymptotics $\Gamma(x) \sim x^{-1}$ as $x \to 0$ all these limits are finite and non-zero, which makes the values $\pm B$ not admissible. This discussion proves formula (5.1.31) for the case in which k and ν have opposite sign. $\qquad \square$

Chapter 6

On Geometric Quantum Confinement in Grushin-type manifolds

In this chapter we present part of the content of my paper [52].It is devoted to the study of the essential self-adjointness of the Laplace-Beltrami operator invariant under the action of a non-compact symmetry group.

6.1 Introduction and main results

We consider the family $\{M_\alpha \equiv (M, g_\alpha) \,|\, \alpha \in [0, +\infty)\}$ of Riemannian manifolds defined by

$$
\begin{aligned}
M &:= \{(x, y) \,|\, x \in \mathbb{R}^+, \, y \in \mathbb{R}\} \\
g_\alpha &:= \mathrm{d}x \otimes \mathrm{d}x + \frac{1}{x^{2\alpha}} \, \mathrm{d}y \otimes \mathrm{d}y \;=\; \mathrm{d}x^2 + \frac{1}{x^{2\alpha}} \, \mathrm{d}y^2 \,.
\end{aligned}
\tag{6.1.1}
$$

The value $\alpha = 1$ selects the standard example of two-dimensional *Grushin manifold* [24, Chapter 11], or *Grushin plane*, and all other members of the above family, as well as of the even larger family defined in (6.1.13) below, will be generically referred to as (two-dimensional) *Grushin-type manifolds*. The value $\alpha = 0$ selects the Euclidean half-plane.

A straightforward computation [2, 16, 92] shows that the Gaussian (sectional) curvature K_α of M_α is

$$
K_\alpha(x, y) \;=\; -\frac{\alpha(\alpha + 1)}{x^2} \,,
\tag{6.1.2}
$$

hence M_α is a hyperbolic manifold whenever $\alpha > 0$.

Each M_α is clearly parallelizable, a global orthonormal frame being

$$
\{X_1, X_2^{(\alpha)}\} \;=\; \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; \begin{pmatrix} 0 \\ x^\alpha \end{pmatrix} \right\} \equiv \left\{ \frac{\partial}{\partial x}, x^\alpha \frac{\partial}{\partial y} \right\}.
\tag{6.1.3}
$$

Remark 6.1.1. Upon extending $\{X_1, X_2^{(\alpha)}\}$ to the whole $\mathbb{R}^2$ with $X_2^{(\alpha)} := \begin{pmatrix} 0 \\ |x|^\alpha \end{pmatrix}$ and defining

$$
\begin{aligned}
M^+ &:= M \,, \qquad M^- := \{(x, y) \,|\, x \in \mathbb{R}^-, \, y \in \mathbb{R}\} \,, \\
\mathcal{Z} &:= \{(0, y) \,|\, y \in \mathbb{R}\} \,,
\end{aligned}
\tag{6.1.4}
$$

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one has now the Lie bracket $[X_1, X_2^{(\alpha)}] = \begin{pmatrix} 0 \\ \alpha|x|^{\alpha-1} \end{pmatrix}$. Thus, if $\alpha = 1$ the fields $X_1, X_2^{(\alpha)}$ define an *almost-Riemannian structure* on $\mathbb{R}^2 = M^+ \cup \mathcal{Z} \cup M^-$, following the notation used in the literature, for a rigorous definition of which we refer, e.g., to [2, Sec. 1] or [93, Sect. 7.1]: the Lie bracket generating condition

$$\dim \mathrm{Lie}_{(x,y)} \mathrm{span}\{X_1, X_2^{(\alpha)}\} \;=\; 2 \qquad \forall (x,y) \in \mathbb{R}^2 \,, \tag{6.1.5}$$

is satisfied in this case. For $\alpha \in (0,1)$ the field $X_2^{(\alpha)}$ is *not* smooth, which prevents $X_1, X_2^{(\alpha)}$ to define an almost-Riemannian structure. However, on $\mathbb{R}^2 \setminus \mathcal{Z}$ the fields $X_1, X_2^{(\alpha)}$ do define a Riemannian structure for every $\alpha \geqslant 0$ given by

$$g_\alpha \;:=\; \mathrm{d}x \otimes \mathrm{d}x + \frac{1}{|x|^{2\alpha}} \, \mathrm{d}y \otimes \mathrm{d}y \,. \tag{6.1.6}$$

To each M_α one naturally associates the Riemannian volume form

$$\mu_\alpha \;:=\; \mathrm{vol}_{g_\alpha} \;=\; \sqrt{\det g_\alpha}\, \mathrm{d}x \wedge \mathrm{d}y \;=\; x^{-\alpha}\, \mathrm{d}x \wedge \mathrm{d}y \,. \tag{6.1.7}$$

By means of (6.1.3) and (6.1.7) one computes

$$\begin{aligned}
X_1^2 &= \frac{\partial^2}{\partial x^2} \,, & \mathrm{div}_{\mu_\alpha} X_1 &= -\frac{\alpha}{x} \,, \\
(X_2^{(\alpha)})^2 &= x^{2\alpha} \frac{\partial^2}{\partial y^2} \,, & \mathrm{div}_{\mu_\alpha} X_2^{(\alpha)} &= 0 \,,
\end{aligned} \tag{6.1.8}$$

whence

$$\begin{aligned}
\Delta_{\mu_\alpha} &= \mathrm{div}_{\mu_\alpha} \circ \nabla \\
&= X_1^2 + X_2^2 + (\mathrm{div}_{\mu_\alpha} X_1)X_1 + (\mathrm{div}_{\mu_\alpha} X_2^{(\alpha)})X_2^{(\alpha)} \\
&= \frac{\partial^2}{\partial x^2} + x^{2\alpha} \frac{\partial^2}{\partial y^2} - \frac{\alpha}{x} \frac{\partial}{\partial x} \,,
\end{aligned} \tag{6.1.9}$$

which is the (Riemannian) Laplace-Beltrami operator on M_α.

In the Hilbert space

$$\mathcal{H}_\alpha \;:=\; L^2(M, \mathrm{d}\mu_\alpha) \,, \tag{6.1.10}$$

understood as the completion of $C_c^\infty(M)$ with respect to the scalar product

$$\langle \psi, \varphi \rangle_\alpha \;:=\; \iint_{\mathbb{R}^+ \times \mathbb{R}} \overline{\psi(x,y)}\, \varphi(x,y) \, \frac{1}{x^\alpha} \, \mathrm{d}x\, \mathrm{d}y \,, \tag{6.1.11}$$

we consider the '*minimal*' free Hamiltonian[1]

$$H_\alpha \;:=\; -\Delta_{\mu_\alpha} \,, \qquad \mathcal{D}(H_\alpha) \;:=\; C_c^\infty(M) \,, \tag{6.1.12}$$

which is a densely defined, symmetric, lower semi-bounded operator (symmetry in particular follows from Green's identity).

Our main question then becomes for which α's the operator H_α is or is not essentially self-adjoint with respect to the Hilbert space $\mathcal{H}_\alpha$, and hence for which α's one has or has not purely geometric quantum confinement in the manifold M_α.

Our main results read as follows.

---

[1]Contrary to the convention adopted in the thesis, in this Appendix the minimal operator is not closed.

Theorem 6.1.2. *If $\alpha \in [0, 1)$, then the operator H_α is not essentially self-adjoint and therefore there is no geometric quantum confinement in the Grushin plane M_α.*

Theorem 6.1.3. *If $\alpha \in [1, +\infty)$, then the operator H_α is essentially self-adjoint and therefore the Grushin plane M_α provides geometric quantum confinement.*

Remark 6.1.4. In the absence of essential self-adjointness, the deficiency index of H_α is *infinite*, as we shall show in the more general Theorem 6.1.6(iii) below. This opens the interesting problem, from the point of view of the quantum-mechanical interpretation, of classifying the self-adjoint extensions of H_α in terms of boundary conditions at the axis $x = 0$, each generating a different dynamics in which the quantum particle 'crosses the boundary'. In such an enormous family of extensions it is of interest, in particular, to discuss those qualified by 'local' boundary conditions, the physically most natural ones. It is not difficult to show, and we intend to discuss these aspects in a follow-up analysis, that the Friedrichs extension satisfies Dirichlet boundary conditions and hence is the distinguished extension that preserves the confinement of the particle. All other extensions drive the particle up to the boundary.

Remark 6.1.5. The lack of geometric quantum confinement in M_α for $\alpha \in [0, 1)$ is compatible with the quantum confinement in *regular* almost-Riemannian structures proved recently in [93, Theorem 7.1]. Indeed, as observed already in Remark 6.1.1, what fails to hold in the first place is the almost-Riemannian structure on $\mathbb{R}^2$ with metric g_α, owing to the non-smoothness of the field $X_2^{(\alpha)}$ in this regime of α.

As is going to emerge in the course of the proofs, our approach has a two-fold feature. On the one hand it is relatively 'rigid', for it does not have an immediate generalisation in application to *generic* almost-Riemannian structures, for which the more versatile, typically perturbative analyses of [16, 93, 44] appear as more efficient and informative. On the other hand, it is particularly 'robust', whenever the problem can be boiled down to a constant-fiber direct integral scheme and to the study of self-adjointness along each fibre, and this allows us to cover a larger class of Grushin planes than that considered so far.

To this aim, let us introduce the manifold $M_f \equiv (M, g_f)$ by replacing (6.1.1) with

$$g_f := \mathrm{d}x \otimes \mathrm{d}x + f^2(x)\,\mathrm{d}y \otimes \mathrm{d}y \qquad (6.1.13)$$

for some measurable function f on $\mathbb{R}$ satisfying

$$
\begin{array}{ll}
\text{(i)} & f(x) > 0 \quad \forall x \neq 0 \\
\text{(ii)} & f(x) \geqslant \kappa \quad \text{in a neighbourhood of } x = 0 \text{ for some } \kappa > 0 \\
\text{(iii)} & f \in C^\infty(\mathbb{R} \backslash \{0\}) \\
\text{(iv)} & 2f(x)f''(x) - f'(x)^2 \geqslant 0 \quad \forall x \neq 0 \,.
\end{array}
\qquad (6.1.14)
$$

The interest in assumptions (6.1.14) is precisely when f becomes singular as $x \to 0$. The reason of condition (iv) will be clarified in due time. The special choice considered above was $f(x) = |x|^{-\alpha}$: in this case condition (iv) reads $\alpha(2 + \alpha)|x|^{-2(1+\alpha)} \geqslant 0$. The smoothness in condition (iii) is required to match the definition of Riemannian manifold, otherwise we shall only use C^2-regularity.

(It is worth mentioning that this point of view, with the more general manifold M_f, is the same as that of [16], and so are formulas (6.1.15)-(6.1.16) below: here in addition we take care of the explicit assumptions (6.1.14) required on f, which finally allow us to prove our general Theorem 6.1.6.)

This yields a generalised Grushin plane with global orthonormal frame

$$\{X_1, X_2^{(f)}\} = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1/f(x) \end{pmatrix} \right\} \equiv \left\{ \frac{\partial}{\partial x}, \frac{1}{f(x)} \frac{\partial}{\partial y} \right\}, \qquad (6.1.15)$$

and a computation analogous to (6.1.7)-(6.1.9) shows that the associated Laplace-Beltrami operator $\Delta_f \equiv \Delta_{\mu_{g_f}}$ ($\mu_{g_f} \equiv \text{vol}_{g_f} = f(x)\,\mathrm{d}x \wedge \mathrm{d}y$) is given by

$$\Delta_f = \frac{\partial^2}{\partial x^2} + \frac{1}{f^2(x)} \frac{\partial^2}{\partial y^2} + \frac{f'(x)}{f(x)} \frac{\partial}{\partial x}\,. \tag{6.1.16}$$

Let us then define the 'minimal' free Hamiltonian

$$H_f := -\Delta_f\,, \qquad \mathcal{D}(H_f) := C_c^\infty(M)\,, \tag{6.1.17}$$

a densely defined, symmetric, lower semi-bounded operator in $\mathcal{H}_f := L^2(M, \mathrm{d}\mu_{g_f})$. The same scheme used for Theorems 6.1.2 and 6.1.3 allows us to discuss the essential self-adjointness of H_f. The result is the following.

Theorem 6.1.6. *Let f be a measurable function satisfying assumptions (6.1.14) and let H_f be the corresponding operator defined in (6.1.17).*

(i) *If, point-wise for every $x \neq 0$,*

$$2ff'' - f'^2 \geqslant \frac{3}{x^2}\,f^2\,, \tag{6.1.18}$$

then H_f is essentially self-adjoint with respect to the Hilbert space $\mathcal{H}_f$, and therefore the generalised Grushin plane M_f produces geometric quantum confinement.

(ii) *If, point-wise for every $x \neq 0$,*

$$2ff'' - f'^2 \leqslant \frac{3-\varepsilon}{x^2}\,f^2 \qquad \text{for some } \varepsilon > 0\,, \tag{6.1.19}$$

then H_f is not essentially self-adjoint, and therefore there is no geometric quantum confinement within the generalised Grushin plane M_f.

(iii) *In case (ii) the operator H_f has infinite deficiency index.*

Remark 6.1.7. Theorem 6.1.6 reproduces Theorems 6.1.2 and 6.1.3 when one makes the special choice $f(x) = x^{-\alpha}$, for in this case

$$2ff'' - f'^2 - \frac{3}{x^2}\,f^2 = \frac{(\alpha-1)(3+\alpha)}{4x^2}\,,$$

whence the threshold value $\alpha = 1$ between absence and presence of confinement. Conditions (6.1.18)-(6.1.19) are homogeneous in f, thus the same conclusion holds for $f(x) = \lambda x^{-\alpha}$, $\lambda > 0$: this amounts to dilate the y-axis, in practice leaving the metric unchanged.

Theorems 6.1.2, 6.1.3, and 6.1.6 are going to be proved in Section 6.3 after an amount of preparation in Section 6.2.

6.2 Technical preliminaries

6.2.1 Unitarily equivalent reformulation

Let us discuss the more general setting of Theorem 6.1.6, that is, the problem of the essential self-adjointness of the minimally defined Laplace-Beltrami operator (6.1.17) in the Hilbert space $L^2(M, \mathrm{d}\mu_{g_f}) = L^2(\mathbb{R}^+ \times \mathbb{R}, f(x)\mathrm{d}x\mathrm{d}y)$.

Through the unitary transformation

$$U_f : L^2(\mathbb{R}^+ \times \mathbb{R}, f(x)\mathrm{d}x\mathrm{d}y) \xrightarrow{\cong} L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}y)\,, \qquad \psi \mapsto f^{1/2}\psi \tag{6.2.1}$$

a simple computation shows that

$$\begin{aligned}
U_f H_f U_f^{-1} &= -\frac{\partial^2}{\partial x^2} - \frac{1}{f^2}\frac{\partial^2}{\partial y^2} + \frac{2ff'' - f'^2}{4f^2} \\
\mathcal{D}(U_f H_f U_f^{-1}) &= C_c^\infty(\mathbb{R}_x^+ \times \mathbb{R}_y).
\end{aligned} \tag{6.2.2}$$

The further unitary $\mathcal{F}_2 : L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}y) \xrightarrow{\cong} L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi)$ consisting of the Fourier transform in the y-variable only produces the operator

$$\mathscr{H}_f := \mathcal{F}_2 U_f H_f U_f^{-1} \mathcal{F}_2^{-1} \tag{6.2.3}$$

whose domain and action are given by

$$\begin{aligned}
\mathscr{H}_f &= -\frac{\partial^2}{\partial x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \\
\mathcal{D}(\mathscr{H}_f) &= \{\psi \in L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi) \,|\, \psi = \mathcal{F}_2 C_c^\infty(\mathbb{R}_x^+ \times \mathbb{R}_y)\}.
\end{aligned} \tag{6.2.4}$$

Thus, for each $\psi \in \mathcal{D}(\mathscr{H}_f)$ the functions $\psi(\cdot, \xi)$ are compactly supported in x inside $(0, +\infty)$ for every ξ, whereas the functions $\psi(x, \cdot)$ are some special case of Schwartz functions for every x.

The particular class of choices $f(x) = x^{-\alpha}$, $\alpha > 0$, yield the operator

$$\begin{aligned}
\mathscr{H}_\alpha &= -\frac{\partial^2}{\partial x^2} + \xi^2 x^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2} \\
\mathcal{D}(\mathscr{H}_\alpha) &= \{\psi \in L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi) \,|\, \psi = \mathcal{F}_2 C_c^\infty(\mathbb{R}_x^+ \times \mathbb{R}_y)\}.
\end{aligned} \tag{6.2.5}$$

The self-adjointness problem for H_f, resp. H_α, is tantamount as the self-adjointness problem for $\mathscr{H}_f$, resp. $\mathscr{H}_\alpha$, and it is this second problem that we are going to discuss.

Remark 6.2.1. The 'potential' (multiplicative) part of $\mathscr{H}_\alpha$, that is, $\frac{\alpha(2+\alpha)}{4x^2}$, is precisely the effective potential V_{eff} introduced in [93] for the study of geometric confinement, computed for the special case of Grushin planes. Whereas in [93] the intrinsic geometric nature of V_{eff} was emphasized, we can here supplement that interpretation by observing that V_{eff} encodes precisely the multiplicative contribution of the original Laplace-Beltrami operator when one transforms unitarily the underlying Hilbert space $L^2(M, \mathrm{d}\mu_g)$, the unitary transformation being $\mathcal{F}_2 \circ U_\alpha$.

For later purposes, let us also mention the following.

Lemma 6.2.2. *The adjoint of $\mathscr{H}_f$ is the operator*

$$\begin{aligned}
\mathscr{H}_f^* &= -\frac{\partial^2}{\partial x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \\
\mathcal{D}(\mathscr{H}_f^*) &= \left\{ \begin{array}{c} \psi \in L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi) \ \textit{such that} \\ \left(-\frac{\partial^2}{\partial x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2}\right)\psi \in L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi) \end{array} \right\}.
\end{aligned} \tag{6.2.6}$$

Proof. $\mathscr{H}_f$ is unitarily equivalent, via Fourier transform in the second variable, to the minimally defined differential operator (6.2.2), whose adjoint is by standard arguments [104, Sect. 1.3.2] the maximally defined realisation of the same differential action, thus with domain consisting of the elements F's such that both F and $\left(-\frac{\partial^2}{\partial x^2} - \frac{1}{f^2}\frac{\partial^2}{\partial y^2} + \frac{2ff'' - f'^2}{4f^2}\right)F$ belong to $L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}y)$. Fourier-transforming such adjoint then yields (6.2.6). $\square$

6.2.2   Constant-fibre direct integral scheme

Whereas obviously $L^2(\mathbb{R}^+_x \times \mathbb{R}_\xi, \mathrm{d}x\mathrm{d}\xi) \cong L^2(\mathbb{R}^+, \mathrm{d}x) \otimes L^2(\mathbb{R}, \mathrm{d}\xi)$, the operator $\mathscr{H}_f$ is not a simple product with respect to the above factorisation, it rather reads as the sum of two products

$$\mathscr{H}_f \;=\; \Big(-\frac{\partial^2}{\partial x^2} + \frac{2ff'' - f'^2}{4f^2} \Big) \otimes \mathbb{1}_\xi + \frac{1}{f^2} \otimes \xi^2 \tag{6.2.7}$$

each of which with the same domain as $\mathscr{H}_f$ itself. The second summand is manifestly essentially self-adjoint on $L^2(\mathbb{R}^+, \mathrm{d}x) \otimes L^2(\mathbb{R}, \mathrm{d}\xi)$, whereas the self-adjointness of the first summand boils down to the analysis of the factor acting on $L^2(\mathbb{R}^+, \mathrm{d}x)$ only, yet there is no general guarantee that the sum of the two preserves the essential self-adjointness.

It is more natural to regard $\mathscr{H}_f$ with respect to the constant-fibre direct integral structure

$$\begin{aligned}
\mathcal{H} \;&:=\; L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\mathrm{d}\xi) \;\cong\; L^2\big(\mathbb{R}, \mathrm{d}\xi\,; L^2(\mathbb{R}^+, \mathrm{d}x)\big) \\
&\equiv\; \int_\mathbb{R}^\oplus \mathrm{d}\xi\, L^2(\mathbb{R}^+, \mathrm{d}x)\,,
\end{aligned} \tag{6.2.8}$$

thus thinking of $L^2(\mathbb{R}^+_x \times \mathbb{R}_\xi, \mathrm{d}x\mathrm{d}\xi)$ as $L^2(\mathbb{R}^+, \mathrm{d}x)$-valued square-integrable functions of $\xi \in \mathbb{R}$. The space $\mathfrak{h} := L^2(\mathbb{R}^+, \mathrm{d}x)$ is the (constant) *fibre* of the direct integral and the scalar products satisfy

$$\langle \psi, \varphi \rangle_\mathcal{H} \;=\; \int_\mathbb{R} \langle \psi(\cdot, \xi), \varphi(\cdot, \xi) \rangle_\mathfrak{h}\, \mathrm{d}\xi\,. \tag{6.2.9}$$

As well known, this is the natural scheme for the multiplication operator form of the spectral theorem [62, Sect. 7.3], as well as for the analysis of Schrödinger's operators with periodic potentials [96, Sect. XIII.16], and we shall exploit this scheme here for the self-adjointness problem of $\mathscr{H}_f$.

For each $\xi \in \mathbb{R}$ we introduce the operator

$$A_f(\xi) \;:=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2}\,, \qquad \mathcal{D}(A_f(\xi)) \;:=\; C_c^\infty(\mathbb{R}^+) \tag{6.2.10}$$

acting on the fibre Hilbert space $\mathfrak{h}$. When $f(x) = x^{-\alpha}$ we write

$$A_\alpha(\xi) \;:=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \xi^2 x^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\,, \quad \mathcal{D}(A_\alpha(\xi)) \;:=\; C_c^\infty(\mathbb{R}^+)\,. \tag{6.2.11}$$

By construction the map $\mathbb{R} \ni \xi \mapsto A_f(\xi)$ has values in the space of densely defined, symmetric operators on $\mathfrak{h}$, in fact all with the *same* domain irrespectively of ξ, and all positive because of the assumptions on f. In each $A_f(\xi)$ ξ plays the role of a fixed parameter. Moreover, all the $A_f(\xi)$'s are closable and each $\overline{A_f(\xi)}$ is positive and with the same dense domain in $\mathfrak{h}$. Arguing as for Lemma 6.2.2 one has

$$A_f(\xi)^* \;=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2}$$

$$\mathcal{D}(A_f(\xi)^*) \;=\; \left\{ \begin{array}{c} \psi \in L^2(\mathbb{R}^+, \mathrm{d}x) \text{ such that} \\ \big(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\xi^2}{f^2} + \frac{2ff''-f'^2}{4f^2} \big)\psi \in L^2(\mathbb{R}^+, \mathrm{d}x) \end{array} \right\}. \tag{6.2.12}$$

Next, with respect to the decomposition (6.2.8) we define the operator B_f in the Hilbert space $\mathcal{H}$ by

$$\mathcal{D}(B_f) \;:=\; \left\{ \psi \in \mathcal{H} \;\middle|\; \begin{array}{ll} \text{(i)} & \psi(\cdot, \xi) \in \mathcal{D}(\overline{A_f(\xi)}) \text{ for almost every } \xi \\ \text{(ii)} & \int_\mathbb{R} \big\| \overline{A_f(\xi)}\psi(\cdot, \xi) \big\|_\mathfrak{h}^2\, \mathrm{d}\xi < +\infty \end{array} \right\} \tag{6.2.13}$$

$$(B_f\psi)(x, \xi) \;:=\; \big(\overline{A_f(\xi)}\, \psi(\cdot, \xi) \big)(x)\,.$$

As customary, for the *whole* (6.2.13) we use the symbol

$$B_f = \int_{\mathbb{R}}^{\oplus} \overline{A_f(\xi)} \, \mathrm{d}\xi. \tag{6.2.14}$$

It can be argued that the fact that the $\overline{A_f(\xi)}$'s have all the same dense domain in $\mathfrak{h}$ guarantees that the decomposition (6.2.14) of B_f is unique and hence unambiguous: if one also had $B_f = \int_{\mathbb{R}}^{\oplus} B_f(\xi) \, \mathrm{d}\xi$ for a map $\xi \mapsto B_f(\xi)$ with $\mathcal{D}(B_f(\xi)) = \mathcal{D}(\overline{A_f(\xi)}) = \mathcal{D}$, a common dense domain in $\mathfrak{h}$, then necessarily $\overline{A_f(\xi)} = B_f(\xi)$ for almost every $\xi \in \mathbb{R}$.

Remark 6.2.3. As suggestive as it would be, it is however important to observe that the operator of interest, $\mathscr{H}_f$, is *not* decomposable as $\mathscr{H}_f = \int_{\mathbb{R}}^{\oplus} A_f(\xi) \, \mathrm{d}\xi$. Indeed, the analogue of condition (i) in (6.2.13) would be satisfied, but condition (ii) would not. More precisely, by definition an element $\psi \in \mathcal{D}(\int_{\mathbb{R}}^{\oplus} A_f(\xi) \, \mathrm{d}\xi)$ does satisfy the property $\psi(\cdot, \xi) \in \mathcal{D}(A_f(\xi)) = C_c^{\infty}(\mathbb{R}^+)$ for every ξ, as is the case for the elements of $\mathcal{D}(\mathscr{H}_f)$, but it also satisfies the property

$$\begin{aligned}
+\infty &> \int_{\mathbb{R}} \left\| A_f(\xi)\psi(\cdot, \xi) \right\|_{\mathfrak{h}}^2 \, \mathrm{d}\xi \\
&= \iint_{\mathbb{R}^+ \times \mathbb{R}} \left| \left(-\frac{\partial^2}{\partial x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \right) \psi(x, \xi) \right|^2 \mathrm{d}x \, \mathrm{d}\xi,
\end{aligned} \tag{6.2.15}$$

and (6.2.15) does not necessarily imply that for every x the function $\psi(x, \cdot)$ is the Fourier transform of a $C_0^{\infty}(\mathbb{R})$-function as it has to be for an element of $\mathcal{D}(\mathscr{H}_f)$. Condition (6.2.15) is surely satisfied by other functions besides all those in $\mathcal{D}(\mathscr{H}_f)$. In fact, the same reasoning proves the (proper) inclusion

$$B_f \supset \mathscr{H}_f. \tag{6.2.16}$$

The operator B_f is not just an extension of $\mathscr{H}_f$, it is a closed symmetric extension.

Proposition 6.2.4 ([92])**.**

(i) B_f *is symmetric.*

(ii) B_f *is closed.*

Proof. Symmetry is immediately checked by means of (6.2.9), thanks to the symmetry of each $\overline{A_f(\xi)}$. Concerning the closedness, let $(\psi_n)_{n \in \mathbb{N}}$, ψ, and Ψ be, respectively, a sequence and two functions in $\mathcal{D}(B_f)$ such that $\psi_n \to \psi$ and $B\psi_n \to \Psi$ in $\mathcal{H}$ as $n \to +\infty$. Thus,

$$\int_{\mathbb{R}} \|\psi_n(\cdot, \xi) - \psi(\cdot, \xi)\|_{\mathfrak{h}}^2 \, \mathrm{d}\xi \xrightarrow{n \to +\infty} 0,$$

$$\int_{\mathbb{R}} \|\overline{A_f(\xi)} \, \psi_n(\cdot, \xi) - \Psi(\cdot, \xi)\|_{\mathfrak{h}}^2 \, \mathrm{d}\xi \xrightarrow{n \to +\infty} 0,$$

which implies that, *up to extracting a subsequence*, and for *almost every* ξ, $\psi_n(\cdot, \xi) \to \psi(\cdot, \xi)$ and $\overline{A_f(\xi)} \, \psi_n(\cdot, \xi) \to \Psi(\cdot, \xi)$ in $\mathfrak{h}$ as $n \to +\infty$. Owing to the closedness of $\overline{A_f(\xi)}$, one must conclude that

$$\psi(\cdot, \xi) \in \mathcal{D}(\overline{A_f(\xi)}) \qquad \text{and} \qquad \overline{A_f(\xi)} \, \psi(\cdot, \xi) = \Psi(\cdot, \xi)$$

for almost every ξ. Therefore,

$$\int_{\mathbb{R}} \left\| \overline{A_f(\xi)} \psi(\cdot, \xi) \right\|_{\mathfrak{h}}^2 \, \mathrm{d}\xi = \|\Psi\|_{\mathcal{H}}^2 < +\infty.$$

Both conditions (i) and (ii) of (6.2.13) are satisfied, which proves that $\psi \in \mathcal{D}(B_f)$ and $B_f \psi = \Psi$, that is, the closedness of B. $\qquad \square$

6.2.3   Self-adjointness of the auxiliary fibred operator

The convenient feature of the auxiliary operator B_f is the possibility of qualifying its self-adjointess in terms of the same property in each fibre.

One direction of this fact is the following application of the well-known property [96, Theorem XIII.85(i)]:

Proposition 6.2.5. *If $A_f(\xi)$ is essentially self-adjoint for each $\xi \in \mathbb{R}$, then B_f is self-adjoint.*

Let us focus on the opposite direction.

Proposition 6.2.6 ([92])**.** *If B_f is self-adjoint, then $A_f(\xi)$ is essentially self-adjoint for almost every $\xi \in \mathbb{R}$.*

Proof. It follows by assumption that for any $\varphi \in \mathcal{H}$ there exists $\psi_\varphi \in \mathcal{D}(B_f)$ with $\varphi = (B_f + \mathrm{i})\psi_\varphi$. Thus, as an identity in $\mathfrak{h}$,

$$\varphi(\cdot, \xi) \;=\; \big(\overline{A_f(\xi)} + i\big)\,\psi_\varphi(\cdot, \xi) \qquad \text{for almost every } \xi\,.$$

In particular, let us run φ over all the $C_c^\infty(\mathbb{R}_x^+ \times \mathbb{R}_\xi)$-functions and let us fix $\xi_0 \in \mathbb{R}$: then obviously $\varphi(\cdot, \xi_0)$ spans the whole space of $C_c^\infty(\mathbb{R}_x^+)$-functions, which is a dense of $\mathfrak{h}$: with this choice the above identity implies that $\mathrm{ran}\overline{(A_f(\xi_0) + i\mathbb{1})}$ is dense in $\mathfrak{h}$ and hence $A_f(\xi_0)$ is essentially self-adjoint. $\square$

In turn, the essential self-adjointness of $A_f(\xi)$ can be now studied by means of very classical methods.

6.2.4   Weyl's analysis in each fibre

Let us re-write

$$A_f(\xi) \;=\; -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W_{\xi,f}\,, \qquad W_{\xi,f}(x) \;:=\; \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2}\,. \tag{6.2.17}$$

Owing to assumptions (6.1.14), $W_{\xi,f}$ is a non-negative continuous function on $\mathbb{R}^+$. With the choice $f(x) = x^{-\alpha}$ it takes the form

$$W_{\xi,\alpha} \;=\; \xi^2 x^{2\alpha} + \frac{\alpha(2+\alpha)}{4x^2}\,. \tag{6.2.18}$$

The essential self-adjointness of $A_f(\xi)$ is controlled by Weyl's limit-point/limit-circle analysis of Section 1.4. Thanks to the continuity and non-negativity of $W_{\xi,\alpha}$, $A_f(\xi)$ is always in the limit point *at infinity* – it suffices to apply Proposition 1.4.4 – so the analysis is boiled down to the sole behaviour *at zero*. Here one has two possibilities:

- if $2ff'' - f'^2 \geqslant 3x^{-2}f^2$, then $W_{\xi,\alpha}(x) \geqslant \frac{3}{4x^2}$, in which case $A_f(\xi)$ is in the limit point at zero (Proposition 1.4.5);

- if instead $2ff'' - f'^2 \leqslant (3-\varepsilon)x^{-2}f^2$ for some $\varepsilon > 0$, since $f^{-2} \leqslant \kappa^{-2}$ around $x = 0$, then $W_{\xi,\alpha}(x) \leqslant \kappa^{-2}\xi^2 + (3-\varepsilon)x^{-2}$, whence also, for some ξ-dependent $\widetilde\varepsilon \in (0,\varepsilon)$, $W_{\xi,\alpha}(x) \leqslant (3-\widetilde\varepsilon)x^{-2}$: in this case $A_f(\xi)$ is in the limit circle at zero (Proposition 1.4.5).

Weyl's criterion presented in Section 1.4 then leads to the following conclusion.

Proposition 6.2.7. *Let $\xi \in \mathbb{R}$ and let f satisfy assumptions* (6.1.14)*.*

(i) If $2ff'' - f'^2 \geqslant 3x^{-2}f^2$, then $A_f(\xi)$ is essentially self-adjoint.

(ii) If $2ff'' - f'^2 \leqslant (3 - \varepsilon)x^{-2}f^2$ for some $\varepsilon > 0$, then $A_f(\xi)$ is not essentially self-adjoint and admits a one-real-parameter family of self-adjoint extensions.

The two alternatives in Proposition 6.2.7 are not mutually exclusive for generic admissible f's, but they are when $f(x) = x^{-\alpha}$, for in this case

$$\frac{2ff'' - f'^2}{4f^2} = \frac{\alpha(2 + \alpha)}{x^2}$$

and the possibilities are only $0 < \alpha < 1$ and $\alpha \geqslant 1$. The conclusion is therefore:

Corollary 6.2.8. *Let $\xi \in \mathbb{R}$. The operator $A_\alpha(\xi)$ is essentially self-adjoint if and only if $\alpha \geqslant 1$.*

6.3 Proofs of the main results

6.3.1 Absence of geometric confinement

We already argued in Section 6.2.1 that it is equivalent to study the essential self-adjointness in $\mathcal{H} = L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}x\,\mathrm{d}\xi)$ of the operator $\mathscr{H}_f$ defined in (6.2.4).

Let us work here in the regime $2ff'' - f'^2 \leqslant (3 - \varepsilon)x^{-2}f^2$ for some $\varepsilon > 0$, or in particular, when $f(x) = x^{-\alpha}$, the regime $\alpha \in (0, 1)$.

Proposition 6.2.7(ii) (in particular, Corollary 6.2.8) then show that for no $\xi \in \mathbb{R}$ can $A_f(\xi)$ be essentially self-adjoint. Owing to Proposition 6.2.6, the auxiliary operator B_f defined in (6.2.13) is not self-adjoint.

On the other hand, B_f is a closed symmetric extension of $\mathscr{H}_f$, owing to (6.2.16) and to Proposition 6.2.4, whence $\overline{\mathscr{H}_f} \subset B_f$.

Now, if $\mathscr{H}_f$ was essentially self-adjoint, it could not be $\overline{\mathscr{H}_f} = B_f$, because this would violate the lack of self-adjointness of B_f. But it could not happen either that B_f is a *proper* extension of $\overline{\mathscr{H}_f}$, because self-adjoint operators are maximally symmetric.

Therefore, $\mathscr{H}_f$ is not essentially self-adjoint. In this regime the Grushin plane does not provide geometric quantum confinement.

Theorems 6.1.2 and 6.1.6(ii) are thus proved.

6.3.2 Presence of geometric confinement

Let us work now in the regime $2ff'' - f'^2 \geqslant 3x^{-2}f^2$, or in particular, when $f(x) = x^{-\alpha}$, the regime $\alpha \in [1, +\infty)$.

Proposition 6.2.7(i) (in particular, Corollary 6.2.8) then shows that for all $\xi \in \mathbb{R}$ the operator $A_f(\xi)$ is essentially self-adjoint, and therefore, owing to Proposition 6.2.5, the auxiliary operator B_f is self-adjoint.

Let us now argue that in the present regime one has

$$\mathscr{H}_f^* \subset B_f. \tag{6.3.1}$$

For (6.3.1) it is sufficient to prove that $\mathcal{D}(\mathscr{H}_f^*) \subset \mathcal{D}(B_f)$, for the differential action of the two operators is the same, as is evident from Lemma 6.2.2.

For generic $F \in \mathcal{D}(\mathscr{H}_f^*)$ formula (6.2.6) gives

$$
\begin{aligned}
+\infty &> \left\| \left(-\frac{\partial^2}{\partial x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \right) F \right\|_{\mathcal{H}}^2 \\
&= \int_{\mathbb{R}} \mathrm{d}\xi \left\| \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\xi^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \right) F(\cdot, \xi) \right\|_{\mathfrak{h}}^2,
\end{aligned}
\tag{*}
$$

whence

$$\left\|\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\xi^2}{f^2}+\frac{2ff''-f'^2}{4f^2}\right)F(\cdot,\xi)\right\|_{\mathfrak{h}}^2 \; < \; +\infty \quad \text{for almost every } \xi\in\mathbb{R}\,.$$

The latter formula, owing to (6.2.12), can be re-written as

$$F(\cdot,\xi) \;\in\; \mathcal{D}(A_f(\xi)^*) \quad \text{for almost every } \xi\in\mathbb{R}$$

and since in the present regime $A_f(\xi)^* = \overline{A_f(\xi)}$, we can also write

$$F(\cdot,\xi) \;\in\; \mathcal{D}(\overline{A_f(\xi)}) \quad \text{for almost every } \xi\in\mathbb{R}\,. \tag{**}$$

Now, (*) and (**) imply that $F\in\mathcal{D}(B_f)$, thus establishing the property (6.3.1).

To complete the argument, let us combine the inclusion $B_f \supset \overline{\mathscr{H}_f}$, that follows from (6.2.16) and from the closedness of B_f, with the inclusion $B_f \subset \overline{\mathscr{H}_f}$, that follows from (6.3.1) by taking the adjoint, because $\overline{\mathscr{H}_f} = \mathscr{H}_f^{**} \supset B_f^* = B_f$, having used the self-adjointness of B_f valid in the present regime. Since then $\overline{\mathscr{H}_f} = B_f$, the conclusion is that $\mathscr{H}_f$ is essentially self-adjoint.

In this regime there is geometric quantum confinement in the Grushin plane. Theorems 6.1.2 and 6.1.6(i) are thus proved.

6.3.3   Infinite deficiency index

When $\mathscr{H}_f$ is *not* self-adjoint, necessarily the spaces $\ker(\mathscr{H}_f^*\pm\mathrm{i}\mathbb{1})$ are non-trivial. Let us show now that in this case

$$\dim\ker(\mathscr{H}_f^*+\mathrm{i}\mathbb{1}) \;=\; \dim\ker(\mathscr{H}_f^*-\mathrm{i}\mathbb{1}) \;=\; \infty\,, \tag{6.3.2}$$

thus proving Theorem 6.1.6(iii).

First, since by assumption each $\overline{A_f(\xi)}$ is not self-adjoint, there exists $\varphi_\xi \in \mathcal{D}(A_f(\xi)^*)$ with $\|\varphi_\xi\|_{\mathfrak{h}}=1$ such that

$$A_f(\xi)^*\,\varphi_\xi \;=\; \mathrm{i}\varphi_\xi\,. \tag{6.3.3}$$

From this we shall now deduce that for any compact interval $J\subset\mathbb{R}$, with $\mathbf{1}_J$ characteristic function of J, the function Φ_J defined by $\Phi_J(x,\xi):=\varphi_\xi(x)\mathbf{1}_J(\xi)$ satisfies

$$\Phi_J \in \mathcal{D}(\mathscr{H}_f^*)\,, \qquad \mathscr{H}_f^*\,\Phi_J \;=\; \mathrm{i}\,\Phi_J\,. \tag{6.3.4}$$

The fact that $\Phi_J \in \mathcal{H}$ follows from $\|\Phi_J\|_{\mathcal{H}}^2 = \int_{\mathbb{R}} \mathrm{d}\xi\,\mathbf{1}_J(\xi)\,\|\varphi_\xi\|_{\mathfrak{h}}^2 = |J|$, where $|J|$ denotes the Lebesgue measure of J. Moreover, for any $\psi\in\mathcal{D}(\mathscr{H}_f)$,

$$\begin{aligned}
\langle\Phi_J,\mathscr{H}_f\psi\rangle_{\mathcal{H}} \;&=\; \iint_{\mathbb{R}^+\times\mathbb{R}} \mathrm{d}x\,\mathrm{d}\xi\,\overline{\varphi_\xi(x)}\mathbf{1}_J(\xi)\,A_f(\xi)\psi(x,\xi) \\
&=\; \int_J \mathrm{d}\xi\,\langle\varphi_\xi,A_f(\xi)\psi(\cdot,\xi)\rangle_{\mathfrak{h}} \;=\; \int_J \mathrm{d}\xi\,\langle A_f(\xi)^*\varphi_\xi,\psi(\cdot,\xi)\rangle_{\mathfrak{h}} \\
&=\; -\mathrm{i}\int_J \mathrm{d}\xi\,\langle\varphi_\xi,\psi(\cdot,\xi)\rangle_{\mathfrak{h}} \;=\; \langle\,\mathrm{i}\,\Phi_J,\psi\rangle_{\mathcal{H}}
\end{aligned}$$

where we used (6.3.3) in the fourth identity, and this establishes precisely (6.3.4).

By the arbitrariness of J, and the obvious orthogonality $\Phi_J \perp \Phi_{J'}$ whenever $J\cap J'=\varnothing$, we have thus produced an infinity of linearly independent eigenfunctions of $\mathscr{H}_f^*$ with eigenvalue i, and the same can be clearly repeated for the eigenvalue $-\mathrm{i}$. This completes the proof of (6.3.2).

6.3.4 Comparison with the compact case

We already mentioned that in [16, Sect. 3.2] and in [17] the closely related problem of geometric quantum confinement was solved in the manifold $\widetilde{M}_\alpha$ – that we can generalise here to

$$\widetilde{M}_f \equiv (\mathbb{R}_x^+ \times \mathbb{T}_y, g_f), \qquad (6.3.5)$$

with the usual g_f from (6.1.13) and f satisfying assumptions (6.1.14).

The compactness of $\mathbb{T}$ trivialises the constant-fibre direct integral scheme: the Fourier transform in the y variable naturally makes the conjugate space an infinite orthogonal direct sum of single-Fourier-mode Hilbert spaces, and our (6.2.4) gets simplified to

$$\mathscr{H}_f = \bigoplus_{k\in\mathbb{Z}} \mathscr{H}_f^{(k)} \qquad (6.3.6)$$

with operators

$$\mathscr{H}_f^{(k)} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{k^2}{f^2} + \frac{2ff'' - f'^2}{4f^2} \qquad (6.3.7)$$

in the fibre Hilbert space $\mathfrak{h} = L^2(\mathbb{R}^+, \mathrm{d}x)$. The continuous variable ξ is thus replaced by the discrete variable k.

In this case the study we made in Section 6.2.3 is not needed: indeed, it is a standard exercise that the essential self-adjointness of $\mathscr{H}_f$ is tantamount as the essential self-adjointness of all the $\mathscr{H}_f^{(k)}$'s, and the latter is fully controlled by Weyl's analysis.

It is worth remarking a noticeable difference between the compact and the non-compact case as far as the essential self-adjointness of the minimally defined Laplace-Beltrami operator is concerned, which emerges when there is *no singularity* in the metric g_f at $x = 0$ – for concreteness, when $f(x) = x^{-\alpha}$ with $\alpha < 0$.

In the 'Grushin cylinder' $M_\alpha = (\mathbb{R}_x^+ \times \mathbb{T}_y, g_\alpha)$, as recently determined in [17, Theorem 1.6], when one considers generic $\alpha \in \mathbb{R}$ it turns out that

- essential self-adjointness holds for $\alpha \in (-\infty, -3] \cup [1, +\infty)$ – this is seen by studying in the usual way each fibre operator $\mathscr{H}_\alpha^{(k)}$ (the analogue of (6.3.7)) and then taking the (analogue of the) infinite orthogonal sum (6.3.6);

- in particular, the lack of essential self-adjointness for $\alpha \in (-3, 1)$ is due to the Fourier mode $k = 0$ only, when $\alpha \in (-3, -1]$, and is due instead to *all* Fourier modes $k \in \mathbb{Z}$ when $\alpha \in (-1, 1)$, that is, in the latter case all $\mathscr{H}_\alpha^{(k)}$'s fail to be essentially self-adjoint on $\mathfrak{h} = L^2(\mathbb{R}^+, \mathrm{d}x)$.

As opposite to that, we can study the same problem in the Grushin plane $M_\alpha = (\mathbb{R}_x^+ \times \mathbb{R}_y, g_\alpha)$ also when $\alpha < 0$ by virtually repeating almost verbatim the analysis of Sections 6.2, 6.3.1, and 6.3.2. Concerning the fibre operator $A_\alpha(\xi)$ on $\mathfrak{h} = L^2(\mathbb{R}^+, \mathrm{d}x)$ we can find that

$$\begin{aligned} \text{if } \alpha \in (-\infty, -1) \cup [1, +\infty), \quad &A_\alpha(\xi) \text{ is ess. self-adj. for almost every } \xi \in \mathbb{R}, \\ \text{if } \alpha = -1, \quad &A_\alpha(\xi) \text{ is ess. self-adj. for } |\xi| \geqslant 1, \\ \text{if } \alpha \in (-1, 1), \quad &A_\alpha(\xi) \text{ is not ess. self-adj.} \end{aligned} \qquad (6.3.8)$$

From (6.3.8), taking the direct integral of the $A_\alpha(\xi)$'s, we conclude that

- essential self-adjointness holds for $\alpha \in (-\infty, -1) \cup [1, +\infty)$;

- the lack of quantum confinement in the complement range $\alpha \in [-1, 1)$ is due to a 'transmission' through the boundary only by the Fourier modes $\xi \in (-1, 1)$ if $\alpha = -1$, and to a transmission by *all* Fourier modes $\xi \in \mathbb{R}$ if $\alpha \in (-1, 1)$.

This shows a difference between the compact and the non-compact case both in the regimes of essential self-adjointness (when $\alpha \in (-3, -1)$ geometric quantum confinement holds in the Grushin plane and not in the Grushin cylinder) and in the Fourier modes responsible for the transmission.

Appendix A

Decomposition of compact homogeneous spaces

This Appendix is a short presentation of the group theory beside Chapter 3. We tried to avoid the introduction of notions that were not strictly necessary for proofs and results that were not important for the purposes of the thesis. The subject is vast and lies in the harmonic analysis on homogeneous spaces. This Appendix is a personal rewriting where I tried to simplify as much as possible the proofs with the unavoidable price of non being optimal in all the statements.

A.1   Basics about Lie Groups

Definition A.1.1. A *Lie group* is a smooth manifold G endowed with a smooth map $: G \times G \to G$ (denoted by $(g_1, g_2) \mapsto g_1 g_2$) that makes G a group, i.e. it satisfies

(i) $\exists e \in G$ such that $eg = ge = g$, $\forall g \in G$;

(ii) $\forall g \in G$, $\exists g^{-1} \in G$ such that $g^{-1}g = gg^{-1} = e$, $\forall g \in G$;

(iii) $g_1(g_2 g_3) = (g_1 g_2)g_3$, for all $g_1, g_2, g_3 \in G$.

It is possible to show that for a Lie group, the map $g \mapsto g^{-1}$ is smooth. Given an element $g \in G$, we can define the *left action* of g as the map $L_g : G \to G$, $L_g g_1 = gg_1$. Similarly we can define the *right action* as a map $R_g : G \to G$, $R_g g_1 = g_1 g$. It is immediate to check that L_g is a smooth map.

If the Lie group is locally compact, then there exists a unique (up to a multiplicative constant) measure which is

(i) inner and outer regular;

(ii) finite on every compact set;

(iii) translational invariant, i.e. for any measurable $A \subset G$ and for every $g \in G$, $\mu(gA) = \mu(A) = \mu(Ag)$.

We recall that given a group G and a set X, an *action* of G on X is a map $\phi : G \times X \to X$ that satisfies

(i) $\phi(e, x) = x$, $\forall x \in X$,

(ii) $\phi(g_1 g_2, x) = \phi(g_1, \phi(g_2, x))$ $\forall g_1, g_2 \in G$ and $x \in X$.

An example of action is the Left action described above, where $X = G$ and $\phi(g_1, g_2) = g_1 g_2$. An action is said *transitive* if X is non-empty and if for each pair $x, y \in X$ there exists $g \in G$ such that $\phi(g, x) = y$.

The above-defined action $\phi : G \times G \to G$ is transitive, as one can see noticing that each element in $G \ni g = \phi(g, e)$.

A classic result by Cartan, also known as 'the closed subgroup theorem' (see [79, Theorem 20.10]), ensures that closed subgroups of a Lie group are smooth submanifolds of the Lie group.

Theorem A.1.2 (E. Cartan). *A closed subgroup $K \subset G$ of a Lie group G is a Lie subgroup of G. K is an embedded submanifold of G.*

Let now K be a closed subgroup of the Lie group G. Let $\pi : G \to G/K$ be the natural projection

$$\pi(g) = [g] = \{g_1 \in [g], \quad \text{iff} \quad \exists h \in K \,|\, gh = g_1\}. \tag{A.1.1}$$

Given G/K the quotient topology, which is the topology in which the map π is continuous, we can endow this space with the structure of a smooth manifold because of the following theorem (the proof can be found, e.g. [79, Theorem 9.22]).

Theorem A.1.3. *If G is a Lie group and K a closed subgroup of G then, with the topology induced by the embedding, the space of left cosets of K in G, G/K, has a natural structure of smooth manifold of dimension $\dim G - \dim K$.*

At this point we see that on the spaces of left cosets G/K we can define naturally an action inherited from the action of G on G. Indeed it is straightforward to check that π commutes with the action of G on G. In this way we can define the action of G on G/K.

Once we endow the quotient space with a smooth structure, we can go ahead and look for a Riemannian structure. The following Theorem goes precisely in this direction.

Theorem A.1.4. *Let G be a Lie group and K a compact subgroup of G. Then the homogeneous space G/K has an invariant Riemannian metric. The volume form associated to the Riemannian structure is an invariant volume form under the action of G on G/K.*

Corollary A.1.5. *G has a left invariant metric.*

Proof. The thesis follows immediately from Theorem A.1.4 by choosing $K = \{e\}$. □

Once a smooth manifold is endowed with a Riemannian metric, the next theorem ensures we can put a Riemannian structure on it.

A.1.1   Representations

Let V be a finite dimensional or separable vector space. We denote with $GL(V)$ the set of all invertible maps from V to V. In case V is a finite dimensional vector space, $GL(V)$ is the general linear group, that is the set of square matrices with non-vanishing determinant. In case V is a separable vector space, $GL(V)$ is the set of all invertible and bounded operators with bounded inverse.

Definition A.1.6. A representation of G on V is a map $\rho : G \to GL(V)$ such that

(i) $\rho(e) = \mathbb{1}$;

(ii) $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$, $\forall g_1, g_2 \in G$;

(iii) $\rho(g^{-1}) = (\rho(g))^{-1}$.

If $\rho : G \to GL(V)$ is a representation, V is called *representation space* and this is a way to define an action on V. A subspace $W \subset V$ of the representation space V is a *representation subspace* if and only if it is invariant under the action of G, which means

$$\rho(g)v \in W \qquad \forall g \in G \qquad \forall v \in W. \qquad \text{(A.1.2)}$$

A representation space is *irreducible* if its only representation subspaces are $\{0\}$ and V. An *irreducible representation* is a representation on an irreducible representation space.

Given two representations of G, $\rho_1 : G \to GL(V_1)$ and $\rho_2 : G \to GL(V_2)$, an *intertwining map* is a map $J : V_1 \to V_2$ which satisfies

$$J\rho_1(g)v = \rho_2(g)Jv \qquad \forall g \in G \qquad \forall v \in V_1. \qquad \text{(A.1.3)}$$

Two representations are said to be *equivalent* if there exists an invertible intertwining map between V_1 and V_2. For the proof of the following standard result in representation theory we refer to standard textbooks on the subjects (e.g. [63, Theorem 4.26]).

Theorem A.1.7 (Shur's lemma). *Let $\rho_1 : G \to GL(V_1)$ and $\rho_2 : G \to GL(V_2)$ be two representations of G and $J : V_1 \to V_2$ an intertwining map. Then*

(i) *If V_1 is irreducible then J is either injective or the zero map;*

(ii) *If V_2 is irreducible then J is either surjective or the zero map;*

(iii) *If V_1 and V_2 are irreducible then J is either an isomorphism or the zero map.*

If $\rho : G \to GL(V)$ is a representation of G on a finite dimensional space V, the *character* of the representation is

$$\chi_\rho(g) = \text{tr}(\rho(g)). \qquad \text{(A.1.4)}$$

The notion of character is important because two equivalent representations have the same characters.

Lemma A.1.8. *If $\rho_1 : G \to GL(V_1)$ and $\rho_2 : G \to GL(V_2)$ are two equivalent finite dimensional representations of G, then $\chi_{\rho_1} = \chi_{\rho_2}$.*

Proof. Since the two representations are equivalent, $J : V_1 \to V_2$ is an isomorphism and from the intertwining property of the map one sees that $\rho_2(g) = J\rho_1(g)J^{-1}$. The thesis follows from the cyclic property of the trace. $\square$

In the case G/K is a smooth manifold, the main goal of the chapter is to show that there exists an orthogonal direct sum decomposition of $L^2(G/K)$ into finite dimensional irreducible representation subspaces. Hence the first step is to consider representations of G on Banach spaces and then to define a natural action of G on $L^p(G/K)$.

Let V be a Banach space with norm $\| \cdot \|_V$. Let $\rho : G \to GL(V)$ be a representation of G on V. We say that ρ is a *strongly continuous representation* if $\forall v \in V$ and $\forall g \in G$, $\rho(g)$ is a bounded linear map from V to V and the function $g \mapsto \rho(g)v$ is continuous in the norm topology. In case V is a Hilbert space, we say that ρ is a *unitary representation* if the operator $\rho(g)$ is unitary for every $g \in G$. We define $L^p(G/K)$ as the spaces (of equivalence classes) of p-integrable functions with respect to the invariant metric of Theorem A.1.4. During this Appendix we always understand L^p spaces with respect to the invariant measure.

Lemma A.1.9. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces, $\rho_1 : G \to GL(\mathcal{H}_1)$ and $\rho_2 : G \to GL(\mathcal{H}_2)$ be two irreducible unitary representations of G and let $B : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ be a map which is antilinear in the first entry and linear in the second one. Assume that for all $g \in G$, $B(\rho_1(g)v_1, \rho_2(g)v_2) = B(v_1, v_2)$ for all $v_1 \in \mathcal{H}_1$ and $v_2 \in \mathcal{H}_2$. Then*

(i) *if $B \neq 0$ then ρ_1 and ρ_2 are equivalent representations;*

(ii) *if ρ_1 and ρ_2 are not equivalent then $B = 0$.*

Proof. The map $v_1 \mapsto B(v_1, \cdot)$ is a map from $\mathcal{H}_1 \to \mathcal{H}_2^*$. Hence, by Riesz representation theorem, to every element $\phi \in \mathcal{H}_2^*$ there exists $w \in \mathcal{H}_2$ such that $\phi(v_2) = \langle w, v_2 \rangle_{\mathcal{H}_2}$ for any $v_2 \in \mathcal{H}_2$. Therefore we define a map $J : \mathcal{H}_1 \to \mathcal{H}_2$ as $v_1 \mapsto w$ where w is the vector associated to $B(v_1, \cdot)$. We now prove that J is an intertwining map. Indeed, for any $v_2 \in \mathcal{H}_2$

$$B(\rho_1(g)v_1, v_2) = B(v_1, \rho_2(g)^{-1}v_2) = \langle w, \rho_2(g^{-1})v_2 \rangle_{\mathcal{H}_2} = \langle \rho_2(g)w, v_2 \rangle_{\mathcal{H}_2}$$

in the last step we used that the representation is unitary, i.e. $\rho_2(g)^* = \rho_2(g^{-1})$. Hence $J\rho_1(g)v_1 = \rho_2(g)Jv_1$. Since by hypothesis $\mathcal{H}_1$ and $\mathcal{H}_2$ are irreducible subspaces, by Shur's lemma (Theorem A.1.7) either J is an isomorphism either J is the zero map. If $B \neq 0$, then J is not the zero map and hence $\mathcal{H}_1$ and $\mathcal{H}_2$ are isomorphic, meaning that ρ_1 and ρ_2 are equivalent.

For (ii), if ρ_1 and ρ_2 are not equivalent then J cannot be an isomorphism and it must be $B = 0$. $\qquad\square$

Definition A.1.10. Let $0 \leqslant p \leqslant \infty$. The *left regular representation* (or simply *regular representation*) λ of G on $L^p(G/K)$ is

$$(\lambda_g f)(x) = f(g^{-1}x). \tag{A.1.5}$$

Before proceeding in the analysis, we put the emphasis on the following theorem which states that the decomposition into finite-dimensional irreducible representation subspaces is a characteristic of compact groups.

Theorem A.1.11. *Let G be a non-compact Lie group and let K be a compact subgroup of G. Then for $1 \leqslant p < \infty$ and for any non-zero $f \in L^p(G/K)$ the set of translates $\{\lambda_g f : g \in G\}$ is infinite dimensional. In particular $L^p(G/K)$ has no nonzero finite dimensional representation subspaces.*

Proof. Since K is compact, we recall that G/K has a G-invariant Riemannian metric. Let $d : G/K \times G/K \to \mathbb{R}^+$ be the distance function defined by the Riemannian metric. If $0 \neq f \in L^p(G/K)$, we can normalise f such that $\|f\|_{L^p(G/K)} = 1$. For $x \in G/K$ and $r > 0$ we denote with $B_x(r) := \{y \in G/K \,|\, d(x,y) < r\}$ the ball of radius r around x. Since G/K is not compact by hypothesis, its diameter - as a metric space - is infinity and thus it is possible to choose a sequence of numbers $r_j < r_{j+1}$ with $r_j \to \infty$ as $j \to \infty$ such that

$$\|f\|_{L^p(B(\pi(e), r_k))} \geqslant 1 - \frac{1}{9^k}$$

which also gives

$$\|f\|_{L^p(G/K \setminus B(\pi(e), r_k))} \leqslant \frac{1}{9^k}.$$

Let now $x_1 = \pi(e)$ and by recursion choose x_{k+1} so that $d(x_{k+1}, \{x_1, \ldots, x_k\}) > 2r_{k+1}$. Choose $g_k \in G$ so that $g_k^{-1}\pi(e) = x_k$ and set $f_k(x) := \lambda_{g_k} f(x) = f(g_k^{-1}x)$ (in this way $f_k(\pi(e)) = f(x_k)$ and with this choice $B_{x_j}(r_j) \not\subseteq B_{x_k}(r_k)$ for $j \neq k$). It follows from the invariance of the measure and the estimates above that for $i \neq j$

$$\|f_i\|_{L^p(B(x_j, r_j))} \leqslant \frac{1}{9^{\min\{i,j\}}}.$$

This implies

$$\sum_{i \neq k}^{+\infty} \|f_i\|_{L^p(B(x_k, r_k))} \leqslant \sum_{i=1}^{+\infty} \frac{1}{9^i} = \frac{1}{10}. \tag{*}$$

By construction, all the f_k's are part of the same representation subspace. Suppose now this subspace to be finite dimensional. This implies that for some set $\{k_1, \ldots, k_m\}$, $f_{k_1}, f_{k_2}, \ldots, f_{k_m}$ are linearly

dependent. Liner dependence implies the existence of a liner relation $\sum_{j=1}^{m} c_j f_{k_j} = 0$ which is non trivial (i.e. not all $c_j = 0$). By reordering we can assume $|c_1| \geqslant c_j$ for all j. Dividing by c_1 we get

$$f_{k_1} = \sum_{i=2}^{+\infty} b_i f_{k_i}$$

with $|b_i| \leqslant 1$. But then

$$\|f_{k_1}\|_{L^p(B(x_{k_1}, r_{k_1}))} = \|f\|_{L^p(B(\pi(e), r_{k_1}))} \geqslant 1 - \frac{1}{9^{k_1}} \geqslant \frac{8}{9},$$

using the inequality (*) together with the fact that $|b_i| \leqslant 1$

$$\|f_{k_1}\|_{L^p(B(x_{k_1}, r_{k_1}))} \leqslant \sum_{i=2}^{+\infty} |b_i| \|f_{k_i}\|_{L^p(B(x_{k_1}, r_{k_1}))} \leqslant \sum_{i \neq k_1} \|f_i\|_{L^p(B(x_{k_1}, r_{k_1}))} \leqslant \frac{1}{10}.$$

And hence we encounter the contradiction $\frac{1}{10} \geqslant \frac{8}{9}$ which completes the proof. $\qquad\square$

Remark A.1.12. The last theorem is false for $p = \infty$. As an example, let $G = \mathbb{R}^n$ and $K = \{0\}$ so that $G/K = \mathbb{R}^n$. Let $0 \neq a \in \mathbb{R}^n$ and set $f_a(x) = e^{ix \cdot a}$ where $\cdot$ denotes the Euclidean scalar product on $\mathbb{R}^n$. Clearly $f_a \in L^\infty(\mathbb{R}^n)$ and $f_a(x+h) = e^{ih \cdot x} f_a(x)$ and thus the one-dimensional space spanned by $f : a$ is invariant under the action of $G = \mathbb{R}^n$ by translation.

We thus see that there is a huge difference in representing compact or non-compact groups. Since in this thesis we decided to focus on compact groups we refer to Appendix 6 for the analysis of a physical system invariant under the action of a non-compact symmetric group. From now on we consider only compact groups.

Proposition A.1.13. *Let G be a group and K a compact Lie subgroup. The regular representation of G on $L^p(G/K)$ acts by isometries for all $1 \leqslant p \leqslant +\infty$:*

$$\|\lambda_g f\|_{L^p(G/K)} = \|f\|_{L^p(G/K)} \tag{A.1.6}$$

Proof. Fix $g \in G$ and $f \in L^p(G/K)$. Then

$$\|\lambda_g f\|_{L^p(G/K)}^p = \int_{G/K} |\lambda_g f(x)|^p \, \mathrm{d}\mu(x) = \int_{G/K} |f(g^{-1}x)|^p \, \mathrm{d}\mu(x)$$
$$= \int_{G/K} |f(y)|^p \, \mathrm{d}\mu(y) = \|f\|_{L^p(G/K)}$$

where we used the change of variables $y = g^{-1}x$ and the invariance of the measure $\mathrm{d}\mu(x) = \mathrm{d}\mu(y)$. $\quad\square$

Corollary A.1.14. *The regular representation on $L^2(G/K)$ acts as unitary operator.*

Proof. From Proposition A.1.13 we know that the regular representation is an isometry from $L^2(G/K)$ into itself. Fix $g \in G$. Then $\lambda_g^{-1} = \lambda_{g^{-1}}$ which means that λ_g is invertible i.e. surjective and injective. Since a surjective isometry is unitary we proved the thesis. $\qquad\square$

Theorem A.1.15. *Let G be a Lie group and K a compact Lie subgroup. For $1 \leqslant p < +\infty$ the regular representation λ of G on $L^p(G/K)$ is strongly continuous.*

Proof. Let $C_0^\infty(G/K)$ be the set of complex-valued smooth functions with compact support on G/K. For any $\varphi \in C_0^\infty(G/K)$, $\lim_{g \to e} \lambda_g \varphi \to \varphi = 0$ uniformly in $x \in G/K$, meaning that

$$\lim_{g \to e} \|\lambda_g \varphi - \varphi\|_{L^p(G/K)} = 0\,.$$

Choose a left invariant metric on G and let $d(g_1, g_2)$ be the Riemannian distance with respect to the chosen invariant metric. Now fix $\varepsilon > 0$ and pick up any $f \in L^p(G/K)$. Then, if $p \in [1, +\infty)$, there is $\varphi \in C_0^\infty(G/K)$ such that

$$\|f - \varphi\|_{L^p(G/K)} < \frac{\varepsilon}{3}\,.$$

Choose now $\delta > 0$ such that if $d(g, e) < \delta$ then

$$\|\varphi - \lambda_g \varphi\|_{L^p(G/K)} < \frac{\varepsilon}{3}\,.$$

For $g \in B_e(\delta)$

$$\|f - \lambda_g f\|_{L^p(G/K)} \leqslant \|f - \varphi\|_{L^p(G/K)} + \|\varphi - \lambda_g \varphi\|_{L^p(G/K)} + \|\lambda_g \varphi - \lambda_g f\|_{L^p(G/K)}$$
$$= 2\|f - \varphi\|_{L^p(G/K)} + \|\varphi - \lambda_g \varphi\|_{L^p(G/K)} < \varepsilon\,.$$

Up to now we proved that λ_g is strongly continuous in e. To extend this result to all the points $g \in G$, let us pick up $g \in G$ and fix $\varepsilon > 0$. For any $g_2 \in B_g(\delta)$, $d(g_1, g_2) < \delta$ and then, using the invariance of the distance, $d(e, g^{-1}g_2) < \delta$. Since λ is an isometry and since the representation is strongly continuous at $e_{,,}$ we can conclude

$$\|\lambda_g f - \lambda_{g_2} f\|_{L^p(G/K)} = \|f - \lambda_{g^{-1}g_2} f\|_{L^p(G/K)} < \varepsilon.$$

Since ε is arbitrary, we completed the proof. $\qquad\square$

A.1.2 Convolution algebra and weakly symmetric spaces

Let $\mathcal{M}_K(G)$ be the set of all measurable functions $f : G/K \times G/K \to \mathbb{C}$ so that for all $x, y \in G/K$ and $g \in G$

$$f(gx, gy) = f(x, y)\,. \tag{A.1.7}$$

For future purposes it is convenient also to define

$$C_K^\infty(G) := \{f \in \mathcal{M}_K(G) : f \in C^\infty(G/K \times G/K)\} \tag{A.1.8}$$

and

$$L_K^p(G/K) := \left\{ f \in \mathcal{M}_K(G) : \int_{G/K} |f(x, \pi(e))|^p \, \mathrm{d}x, \ \int_{G/K} |f(\pi(e), y)|^p \, \mathrm{d}y < +\infty \right\} \tag{A.1.9}$$

and we notice that $L_K^p(G/K)$ is a normed space once one defines the norm

$$\|f\|_{L_K^p(G)} := \max \left\{ \|f(\cdot, \pi(e))\|_{L^p(G/K)}, \|f(\pi(e), \cdot)\|_{L^p(G/K)} \right\} \tag{A.1.10}$$

As a consequence of the invariance of the measure one can prove that

$$\int_{G/K} |f(x, y)|^p \, \mathrm{d}y = \int_{G/K} |f(\pi(e), y)|^p \, \mathrm{d}y\,, \tag{A.1.11}$$

$$\int_{G/K} |f(x, y)|^p \, \mathrm{d}x = \int_{G/K} |f(x, \pi(e))|^p \, \mathrm{d}x\,. \tag{A.1.12}$$

We also warn that, at this level of generality, the finiteness of one of the two integrals in (A.1.9) does not imply the finiteness of the other one.

We will need in the following, the class of integral operators defined from functions in $L_K^p(G)$. Given $h \in L_K^1(G)$, we define the operator $T_h : L^p(G/K) \to L^p(G/K)$ by

$$(T_h f)(x) := \int_{G/K} h(x,y) f(y) \, dy. \tag{A.1.13}$$

Lemma A.1.16. *Let $h \in L_K^1(G)$. Then $T_h : L^p(G/K) \to L^p(G/K)$ is a bounded linear operator with*

$$\|T_h f\|_{L^p(G/K)} \leqslant \|h\|_{L_K^1(G)} \|f\|_{L^p(G/K)}. \tag{A.1.14}$$

Proof. We denote with p' the dual of p, which is $\frac{1}{p} + \frac{1}{p'} = 1$. We first estimate:

$$
\begin{aligned}
|(T_h f)(x)| &\leqslant \int_{G/K} |h(x,y)| \, |f(y)| \, dy \\
&= \int_{G/K} |h(x,y)|^{\frac{1}{p'}} |h(x,y)|^{\frac{1}{p}} |f(y)| \, dy \\
&\leqslant \left(\int_{G/K} |h(x,y)| \, dy \right)^{\frac{1}{p'}} \left(\int_{G/K} |h(x,y)| \, |f(y)|^p \, dy \right)^{\frac{1}{p}} \\
&= \|h\|_{L_K^1(G)}^{\frac{1}{p'}} \left(\int_{G/K} |h(x,y)| \, |f(y)|^p \, dy \right)^{\frac{1}{p}}.
\end{aligned}
$$

where in the third step we used Hölder inequality.

$$
\begin{aligned}
\|T_h f\|_{L^p(G/K)}^p &= \int_{G/K} |T_h f)(x)|^p \, dx \\
&\leqslant \|h\|_{L_K^1(G)}^{\frac{p}{p'}} \int_{G/K} |h(x,y)| \int_{G/K} |f(y)|^p \, dy \, dx \\
&= \|h\|_{L_K^1(G)}^{\frac{p}{p'}} \|h\|_{L_K^1(G)} \|f\|_{L^p(G/K)}^p
\end{aligned}
$$

which proves the thesis. $\square$

Lemma A.1.17. *Let $h \in L_K^1(G)$, then the integral operator T_h commutes with the action of G:*

$$T_h \circ \lambda_g = \lambda_g \circ T_h \tag{A.1.15}$$

for all $g \in G$.

Proof. Let $f \in L^p(G/K)$, then

$$
\begin{aligned}
(T_h \circ \lambda_g f)(x) &= \int_{G/K} h(x,y) f(g^{-1}y) \, dy \\
&= \int_{G/K} h(x,gy) f(y) \, dy \qquad (y \mapsto gy) \\
&= \int_{G/K} h(g^{-1}x, y) f(y) \, dy \qquad (h(x,gy) = h(g^{-1}x, g^{-1}gy)) \\
&= (\lambda_g \circ T_h f)(x).
\end{aligned}
$$

$\square$

A function $f : G \to \mathbb{C}$ is said to be *isotropic* with respect to K if $f(ax) = f(x)$ for all $a \in K$ and for all $x \in G$. If E is a representation space of functions, we denote by E^K the set of all isotropic function on E, that is E^K is the set of all invariant elements of E under the action of K.

Let $\mathcal{M}(G/K)^K$ be the set of measurable isotropic functions on G/K. We define the restriction operator

$$\text{Res} : \mathcal{M}_K(G) \to \mathcal{M}(G/K)^K \tag{A.1.16}$$

by

$$(\text{Res}\, h)(x) := h(x, \pi(e)). \tag{A.1.17}$$

Note that if $a \in K$, $(\text{Res}\, h)(ax) = h(ax, \pi(e)) = h(ax, \pi(ae)) = h(x, \pi(e)) = (\text{Res}\, h)(x)$ and therefore Res is a well defined map.

Sometimes one refers to the above-mentioned restriction map as the 'left restriction'. It is possible to define a right restriction aswell as $(\text{RRes}\, h)(y) = h(\pi(e), y)$. For a reason that will be clear in few pages, for our purposes it is enough to have the above-defined restriction function.

As opposite to the restriction function, we define the *extension* of a function in $\mathcal{M}(G/K)^K$ as

$$\text{Ext} : \mathcal{M}(G/K)^K \to \mathcal{M}_K(G) \tag{A.1.18}$$

by

$$(\text{Ext}\, h)(x, y) = h(\eta^{-1}x) \qquad \text{with}\, \eta \in G \quad \text{s.t.} \quad \eta\pi(e) = y. \tag{A.1.19}$$

We have now to check that the definition does not depend on the choice of η. Indeed, let η_1 be another element in G such that $\eta_1\pi(e) = y$. Then, by definition, $\eta_1 = \eta a$ for some element $a \in K$ and since h is isotropic

$$f(\eta_1^{-1}x) = f(a^{-1}\eta^{-1}x) = f(\eta^{-1}x). \tag{A.1.20}$$

Restriction and extension map are one the inverse of the other, as it is shown by the following computation

$$(\text{Ext}\,\text{Res}\, h)(x, y) = (\text{Res}\, h)(\eta^{-1}x) = h(\eta^{-1}x, \pi(e)) = h(x, \eta\pi(e)) = h(x, y). \tag{A.1.21}$$

Moreover, it follows by definition that

$$\|\text{Ext}\, f\|_{L^p_K(G)} = \|f\|_{L^p(G/K)}. \tag{A.1.22}$$

We now use convolutions to construct smoothing operators. Let us define a function $\varphi : \mathbb{R} \to \mathbb{R}^+$ such that $\text{supp}\,\varphi \subset [-1, 1]$. For $\delta > 0$ we define

$$\varphi_\delta(x, y) := C(\delta)\varphi(\delta^{-2}d(x, y)^2) \tag{A.1.23}$$

where $C(\delta)$ is chosen to satisfy

$$\int_{G/K} \varphi_\delta(x, \pi(e))\, \mathrm{d}x = 1. \tag{A.1.24}$$

It is possible to see directly from the definition that φ_δ has the following properties:

(i) $\varphi_\delta(gx, gy) = \varphi_\delta(x, y)$

(ii) $\varphi_\delta(x, y) = \varphi_\delta(y, x)$

(iii) $\varphi_\delta(x, y) = 0$ of $d(x, y) \geqslant \delta$

(iv) $\varphi_\delta \in C^\infty(G/K \times G/K)$ for δ small enough

(v) $\varphi_\delta(x, y) \geqslant 0$.

Theorem A.1.18. *Let $f \in L^p_{loc}(G/K)$ and define f_δ by*

$$f_\delta(x) := (T_{\varphi_\delta} f)(x) = \int_{G/K} \varphi_\delta(x, y) f(y) \, \mathrm{d}y. \tag{A.1.25}$$

For small δ, $f_\delta \in C^\infty(G/K)$, $\lim_{\delta \downarrow 0} f_\delta(x) = f(x)$ for almost every $x \in G/K$. If $1 \leqslant p < \infty$ and $f \in L^p(G/K)$, then $\lim_{\delta \downarrow 0} \|f - f_\delta\|_{L^p(G/K)} = 0$. If $f \in C^k(G/K)$ for some $k \geqslant 0$ then $f_\delta \to f$ in the C^k topology uniformly on compact subsets of G/K.

Definition A.1.19. An homogeneous space G/K with K compact is said to be *weakly symmetric* if $h \in \mathcal{M}_K(G)$ implies $h(x, y) = h(y, x)$ for almost every $x, y \in G/K$.

Since in the second part of the thesis we deal with homogeneous spaces of the form $\mathbb{S}^n$ we recall the following well known result.

Proposition A.1.20. *The sphere $\mathbb{S}^n = SO(n+1)/SO(n)$ is a weakly symmetric space.*

Proposition A.1.21. *If G/K is weakly symmetric then the norms on the spaces $L^p_K(G)$ are given by*

$$\|h\|_{L^p_K(G)} = \left(\int_{G/K} |h(x, \pi(e))|^p \, \mathrm{d}x \right)^{\frac{1}{p}} = \left(\int_{G/K} |h(\pi(e), y)|^p \, \mathrm{d}y \right)^{\frac{1}{p}}. \tag{A.1.26}$$

Also the convolution algebra is commutative, meaning that $\forall h, k \in L^1_K(G)$ $h * k = k * h$.

Proof. Equality of norms (A.1.26) follows directly from the fact that $h(x, y)$ is measurable and hence, since the space is weakly symmetric, $h(x, y) = h(y, x)$ whence the equalities of the two norms in (A.1.9).

To see that the convolution algebra is commutative

$$
\begin{aligned}
(h * k)(x, y) &= \int_{G/K} h(x, z) \, k(z, y) \, \mathrm{d}z \\
&= \int_{G/K} k(z, y) \, h(x, z) \, \mathrm{d}z && \text{symmetry of } h, k \\
&= \int_{G/K} k(y, z) h(z, x) \, \mathrm{d}z \\
&= (k * h)(y, x) && k * h \text{ is measurable and hence symmetric} \\
&= (h * k)(x, y)
\end{aligned}
$$

from which the conclusion follows. $\qquad\square$

Lemma A.1.22. *If G/K is compact, then $L^2_K(G)$ is closed under the convolution product $(f, g) \mapsto f * g$ and for all functions $h \in L^2_K(G)$, the integral operator $T_h : L^2(G/K) \to L^2(G/K)$ is compact.*

Proof. Let $f, g \in L^2_K(G)$. By Cauchy-Schwartz inequality

$$
\begin{aligned}
\int_{G/K} |(f * g)(x, \pi(e))|^2 \, \mathrm{d}x &\leqslant \int_{G/K} \left(\int_{G/K} |f(x, z) g(z, \pi(e))| \, \mathrm{d}z \right)^2 \mathrm{d}x \\
&\leqslant \int_{G/K} \left(\int_{G/K} |f(x, z)|^2 \, \mathrm{d}z \right) \left(\int_{G/K} |g(y, \pi(e))|^2 \, \mathrm{d}y \right) \mathrm{d}x \\
&= \mu(G/K) \|f\|_{L^2_K}^2 \|g\|_{L^2_K}^2.
\end{aligned}
$$

Thus $f * g$ is in $L^2_K(G)$. To prove that the operator is compact we prove that it is Hilbert-Schmidt. Indeed

$$\int_{G/K \times G/K} |h(x,y)|^2 \, \mathrm{d}x \mathrm{d}y = \int_{G/K} \|h\|^2_{L^2_K} \, \mathrm{d}y = \mu(G/K)\|h\|^2_{L^2_K}$$

and this completes the proof. $\qquad\square$

Proposition A.1.23. *Let G/K be a weakly symmetric space. Then for $1 \leqslant p \leqslant +\infty$ there are Banach space isomorphisms* Res *and* Ext *given by (A.1.16)-(A.1.17) and (A.1.18)-(A.1.19).*

Proof. The statement is a straightforward consequence of how Ext and Res are defined together with (A.1.22). $\qquad\square$

A.1.3   Decomposition of representations

Proposition A.1.24. *Let G be a compact group and $\mathcal{H}$ be a Hilbert space with inner product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$. Assume that $\rho : G \to GL(\mathcal{H})$ is a strongly continuous representation of G on $\mathcal{H}$. Then there is a inner product $(\cdot,\cdot)$ which is*

(i) *invariant under G,*

(ii) *equivalent to $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ in the sense that there exists a positive constant for which $\frac{1}{c}\|x\|_{(\cdot,\cdot)} \leqslant \|x\|_{\langle\cdot,\cdot\rangle} \leqslant c\|x\|_{(\cdot,\cdot)}$.*

Proof. One defines

$$(x,y) := \int_G \langle\rho(g)x,\rho(g)y\rangle_{\mathcal{H}} \, \mathrm{d}g\,.$$

The properties of the inner product descend from the properties of the inner product $\langle\cdot,\cdot,\rangle_{\mathcal{H}}$ and the existence of the constant depend on the volume of G. $\qquad\square$

Lemma A.1.25. *Let G be a compact group, $\mathcal{H}$ a Hilbert space and $\rho : G \to GL(\mathcal{H})$ and assume that the inner product is invariant under G. If E is a representation subspace for G on $\mathcal{H}$, so is $E^\perp$.*

Proof. Let $x \in E^\perp$ and pick up $g \in G$. $\forall y \in E$

$$0 = \langle\rho(g)x,y\rangle = \langle\rho(g^{-1})\rho(g)x,\rho(g^{-1})y\rangle = \langle x,\rho(g^{-1})y\rangle$$

whence we proved that $\rho(g^{-1})y \in E^\perp$. The arbitrariness of x,g and y led to the proof of the Lemma. $\qquad\square$

Lemma A.1.26. *Let $\rho : G \to GL(\mathcal{H})$ be a strongly continuous representation of G in $\mathcal{H}$. Then, for any $v \in \mathcal{H}$, $f_v(g) : G \to \mathbb{C}$, $g \mapsto f_v(g) := \langle v,\rho(g)v\rangle$ is a continuous function.*

Proof. Using Cauchy-Schwarz inequality and strong continuity we get

$$\begin{aligned}
|f_v(g_1) - f_v(g_2)| &= |\langle v,(\rho(g_1) - \rho(g_2))v\rangle| \\
&\leqslant \|v\|\|(\rho(g_1) - \rho(g_2))v\| \leqslant C\,d(g_1,g_2)\,\|v\|^2\,.
\end{aligned}$$

It is immediate to see that if we fix $\varepsilon > 0$, there exists $0 < \delta := \frac{\varepsilon}{2C\,\|v\|^2}$ such that if $d(g_1,g_2) < \delta$ then $|f(g_1) - f(g_2)| < \varepsilon$. $\qquad\square$

Lemma A.1.27. *Let $\rho : G \to GL(\mathcal{H})$ be a strongly continuous representation of the compact group G on $\mathcal{H}$ endowed with a G-invariant scalar product. Then there exists a finite dimensional representation subspace $E \subset \mathcal{H}$.*

Proof. The idea of the proof is to find a compact self-adjoint linear operator on $\mathcal{H}$ which commutes with the action of G and then to find the required representation subspace as one of the eigenspaces of such a self-adjoint operator.

Let $0 \neq v \in V$. We can assume $\|v\|_{\mathcal{H}} = 1$. Then we define

$$Ax := \frac{1}{\mu(G)} \int_G P_{\rho(g)v} x \, dg$$

where $P_{\rho(g)v}$ is the orthogonal projector onto $\rho(g)v$. We now prove that $\|Ax\| \leq \|x\|$ for all $x \in \mathcal{H}$.

$$\|Ax\|_{\mathcal{H}} \leq \frac{1}{\mu(G)} \int_G \|P_{\rho(g)v} x\|_{\mathcal{H}} \, dg \leq \sup_{g \in G} \|P_{\rho(g)} x\|_{\mathcal{H}} \leq \|x\|_{\mathcal{H}} .$$

As a second step we show that A commutes with the action of G. Indeed

$$
\begin{aligned}
A\rho(g)x &= \frac{1}{\mu(G)} \int_G \langle \rho(g)x, \rho(h)v \rangle \, \rho(h)v \, dh \\
&= \frac{1}{\mu(G)} \int_G \langle x, \rho(g)^* \rho(h)v \rangle \, \rho(h)v \, dh \\
&= \frac{1}{\mu(G)} \int_G \langle x, \rho(g^{-1}h)v \rangle \, \rho(g)\rho(g^{-1}h)v \, dh \\
&= \frac{1}{\mu(G)} \int_G \langle x, \rho(g^{-1}h)v \rangle \, \rho(g)\rho(g^{-1}h)v \, d(g^{-1}h) = \rho(g)Ax .
\end{aligned}
$$

We now prove that A is self-adjoint. Since it is bounded, it is sufficient to show that it is symmetric.

$$
\begin{aligned}
\langle Ax, y \rangle &= \frac{1}{\mu(G)} \left\langle \int_G P_{\rho(g)v} x \, dg, y \right\rangle = \frac{1}{\mu(G)} \int_G \langle P_{\rho(g)v} x, y \rangle \, dg \\
&= \frac{1}{\mu(G)} \int_G \langle x, P_{\rho(g)v} y \rangle \, dg = \left\langle x, \frac{1}{\mu(G)} \int_G P_{\rho(g)v} y \, dg \right\rangle = \langle x, Ay \rangle .
\end{aligned}
$$

To show that A is not the null operator we exploit the equality

$$
\begin{aligned}
\langle Av, v \rangle &= \frac{1}{\mu(G)} \int_G \langle v, \rho(g)v \rangle \langle \rho(g)v, v \rangle \, dg \\
&= \frac{1}{\mu(G)} \int_G |\langle v, \rho(g)v \rangle|^2 \, dg .
\end{aligned}
$$

We now prove that, as a consequence of Lemma A.1.26, the last quantity is strictly positive. Indeed, for $g = e$, $|\langle \rho(g)v, v \rangle| = 1$ and therefore for $\varepsilon > 0$ small enough

$$
\begin{aligned}
\frac{1}{\mu(G)} \int_G |\langle \rho(g)v, v \rangle|^2 \, dg &\geq \frac{1}{\mu(G)} \int_{B_e(\delta)} |\langle \rho(g)v, v \rangle|^2 \, dg \\
&\geq (1 - \varepsilon) \frac{\mu(B_e(\delta))}{\mu(G)} > 0
\end{aligned}
$$

We now prove that A is compact. Let $\| \cdot \|_{op}$ be the operator norm. It is a standard result (see e.g. [125, Theorem 1.18]) that if an operator can be approximated in operator norm by finite rank operators then it is compact.

Since the group G is compact, there is a finite cover $\{U_1, \ldots, U_m\}$ of G so that if $g_1, g_2 \in U_i$ then $d(g_1, g_2) < \delta$. By strong continuity of the representation, this implies that $\|(\rho(g_1) - \rho(g_2))v\| < \varepsilon$. For each i, choose $g_i \in U_i$ and let $\{\varphi_i\}_{i=1}^m$ be a partition of unity subordinate to the cover $\{U_i\}_{i=1}^m$. We define a linear operator

$$A_i x = \frac{1}{\mu(G)} \int_G \varphi_i(h) P_{\rho(h)v} x \, dh .$$

By construction $A = \sum_{i=1}^{m} A_i$. We now define a rank one operator by

$$B_i x \ := \ \frac{1}{\mu(G)} \int_G \varphi(h) \langle \rho(h)v, x \rangle \, \rho(g_i)v \, \mathrm{d}h$$

and a finite rank operator

$$B \ := \ \sum_{i=1}^{m} B_i \, .$$

If g is in the support of φ_i, then both g and g_i are in U_i and thus $\|\rho(g)v - \rho(g_i)v\| < \varepsilon$. As $\varphi_i(g)$ vanishes for all g not in the support of φ_i and $\|\rho(g)v\| = 1$

$$\|\langle \rho(h)v, x \rangle \varphi_i(h) \rho(g_i)v - \langle \rho(h)v, x \rangle \rho(h)v \| \varphi_i(h)$$
$$= |\langle \rho(h)v, x \rangle| \, \|\rho(g_i)v - \rho(h)v\| \varphi_i(h) \leqslant \varepsilon \|x\| \varphi_i(h)$$

and hence

$$\|A_i x - B_i x\| \leqslant \frac{1}{\mu(G)} \int_G \|\langle \rho(h)v, x \rangle \varphi_i(h) \rho(g_i)v - \langle \rho(h)v, x \rangle \rho(h)v \| \varphi_i(h) \, \mathrm{d}h$$
$$\leqslant \varepsilon \|x\| \frac{1}{\mu(G)} \int_G \varphi_i(h) \, \mathrm{d}h$$

and hence

$$\|Ax - Bx\| \leqslant \sum_{i=1}^{m} \|A_i x - B_i x\| \leqslant \varepsilon \|x\| \sum_{i=1}^{m} \frac{1}{\mu(G)} \int_G \varphi_i(h) \, \mathrm{d}h = \varepsilon \|x\| \, .$$

which implies $\|A - B\|_{op} < \varepsilon$. As ε was arbitrary, this show that A can be approximated by finite rank operators and completes the proof that A is compact.

We proved that A is a compact operator different from zero an hence it has at least one non-zero eigenvalue α. Let E_α be the corresponding eigenspace. If $x \in E_\alpha$ then, by construction, $\rho(g)Ax = A\rho(g)x \in E_\alpha$. Thus E_α is a representation subspace of $\mathcal{H}$. Since A is compact and $\alpha \neq 0$ the space E_α is finite dimensional. Let now E be a representation subspace of minimal dimension, then E is a finite dimensional irreducible representation subspace of $\mathcal{H}$. □

A.2   Decomposition of $L^2(G/K)$

Theorem A.2.1. *Let $\rho : G \to GL(\mathcal{H})$ be a strongly continuous representation of the compact group G on the Hilbert space $\mathcal{H}$ and assume that the inner product $\langle \cdot, \cdot \rangle$ is invariant under the action of G. Then $\mathcal{H}$ is an orthogonal direct sum*

$$\mathcal{H} \ = \ \bigoplus_{\alpha \in A} E_\alpha \tag{A.2.1}$$

of finite dimensional irreducible representation spaces E_α.

Proof. Let A be the set of indices for which $\alpha \in A$ if and only if $E_\alpha \subset \mathcal{H}$ is a finite dimensional representation subspace for G on $\mathcal{H}$ with $E_\alpha \perp E_\beta$ if $\alpha \neq \beta$. Let $\mathscr{E} := \{E_\alpha, \alpha \in A\}$ and let $\mathscr{B} = \mathscr{P}(\mathscr{E})$ is the set of parts of $\mathscr{E}$. From Lemma A.1.27 we know that $A \neq \varnothing$ and hence $\mathscr{B}$ is not empty. We now order $\mathscr{B}$ by inclusion, i.e. if $F_1, F_2 \in \mathscr{B}$ we write $F_1 < F_2$ if and only if $F_1 \subset F_2$. Let C be a totally ordered subset of $\mathscr{B}$. It has a majorant which is $F_{maj} = \bigcup_{\alpha : E_\alpha \in C} \{E_\alpha\}$. We are hence in the condition of applying Zorn's Lemma and hence $\mathscr{B}$ has a maximal element, F_{max}. Denoting $E = \bigoplus_{\alpha : E_\alpha \in F_{max}} E_\alpha$, if $E \neq \mathcal{H}$ then $E^\perp$ is a representation subspace of $\mathcal{H}$ and it has a finite dimensional representation subspace E_γ. This implies $E_\gamma \in \mathscr{E}$ and $F_{max} \cup \{E_\gamma\} \in \mathscr{B}$ contradicting the maximality of F_{max}. □

Corollary A.2.2. *Let G be a compact Lie group and K a closed subgroup of G. Then there is an orthogonal direct sum*

$$L^2(G/K) = \bigoplus_{\alpha \in A} E_\alpha \tag{A.2.2}$$

where each E_α is finite dimensional irreducible representation subspace of $L^2(G/K)$ under the regular representation $(\lambda_g f)(x) = f(g^{-1}x)$.

Up to now we proved that the space of square integrable functions on a homogeneous space decomposes into an orthogonal direct sum of finite dimensional spaces. To set precisely the decomposition we need to answer two more questions: which subspaces E_α are present in the decomposition and with which multiplicity.

Proposition A.2.3. *Let G be a compact group and $\rho : G \to GL(V)$ be a finite dimensional representation of G. Then $L^2(G)$ contains a representation subspace of G isomorphic to V.*

Proof. Fix any nonzero vector $v_0 \in V$ and define a function $\varphi : E \to L^2(G)$. Recalling that an element in $L^2(G)$ is a function from $G \to \mathbb{C}$, we set

$$(\varphi(v))(\cdot) := \langle v, \rho(\cdot)v_0 \rangle.$$

Clearly $\varphi(v) : G \to \mathbb{C}$ and is linear in v. Moreover it is an intertwining map

$$\varphi(\rho(g)v)(x) = \langle \rho(g)v, \rho(x)v_0 \rangle = \langle v, \rho(g^{-1}x)v_0 \rangle = \lambda_g(\varphi(v))(x).$$

Therefore $\lambda_g \circ \varphi = \varphi \circ \rho_g$. Since $\varphi(v_0)(e) = \langle v_0, v_0 \rangle \neq 0$, φ is not the zero map and hence, by Shur's lemma (Theorem A.1.7), $\varphi : V \to \varphi(V)$ is an isomorphism. Hence $E := \varphi(V)$ is the representations subspace of G on $L^2(G)$ isomorphic to V. $\qquad\square$

Proposition A.2.4. *Let G be a compact group and H be a closed subgroup of G. Let V be an irreducible finite dimensional representation subspace. Then $L^2(G/K)$ has a representation subspace isomorphic to V if and only if $V^K \neq \{0\}$.*

Proof. By hypothesis there exists a nonzero vector $v_0 \in V^K$. We define a function $\varphi : E \to L^2(G/K)$,

$$(\varphi(v))(\cdot) := \langle v, \rho(\pi^{-1}(\cdot))v_0 \rangle.$$

We have to show that the definition does not depend on the element on the fibre of $\pi^{-1}(x)$ for $x \in G/K$. Let g_1 and g_2 be two elements such that $\pi(g_1) = \pi(g_2)$. Then there exists $k \in K$ such that $g_1 k = g_2$. The definition is well posed since, using the isotropy of v_0, we see

$$\langle v, \rho(g_1)v_0 \rangle = \langle v, \rho(g_1 k)\rho(k^{-1})v_0 \rangle = \langle v, \rho(g_2)v_0 \rangle$$

Repeating verbatim the argument of the previous proposition gives the 'if' direction of the thesis.

For the 'only if' let us suppose that $L^2(G/K)$ has a finite dimensional representation subspace isomorphic to V. Since G/K has an invariant Riemannian metric we denote with $d(x, y)$ the Riemannian distance between $x, y \in G/K$. Let $B_x(r)$ the ball of radius r around x.

Since $V \neq \{0\}$ then there exists $f_0 \in V$ and $B_{x_0}(r)$ such that $\int_{B_{x_0}(r)} f_0(x) \, dx \neq 0$ (if the integral were equal to zero for every ball, then $f_0(x) = 0$ for almost every x). We can now define a linear functional $\lambda : V \to \mathbb{C}$, $\lambda(f) := \int_{B_{x_0}(r)} f(x) \, dx$. Since V is a finite dimensional vector space, by Riesz representation theorem there exists a vector $h \in V$ such that, for all $f \in V$, $\Lambda(f) = \langle h, f \rangle$. Since $\Lambda(f_0) \neq 0$, we know that Λ is not the zero map and $h \neq 0$. Moreover, for all $k \in K$, $\int_{B_{x_0}(r)} (\lambda_k f)(x) \, dx = \int_{B_{x_0}(r)} f(x) \, dx$ because the measure is invariant under the action of $k \in K \subset G$ and $B_{x_0}(r) = B_{kx_0}(r)$. Since $\Lambda(\lambda_k f) = \Lambda(f)$, this implies also that $h(x) = (\lambda_k h)(x)$ and then $h \in V^K$ completing the proof. $\qquad\square$

Let $\mathscr{A}$ be the set of linear functionals $\alpha : L_K^2(G) \to \mathbb{C}$ such that the space

$$E_\alpha \; := \; \{f \in L^2(G/K) \; : \; T_h f = \alpha(h)f \quad \forall h \in L_K^2(G)\} \tag{A.2.3}$$

is non-zero.

Theorem A.2.5. *Let G/K be a compact space for which the convolution algebra is commutative. Let $\mathscr{A}$ be as above. Then*

$$L^2(G/K) \; = \; \bigoplus_{\alpha \in \mathscr{A}} E_\alpha \tag{A.2.4}$$

(i) Each E_α is a representations subspace of $L^2(G/K)$;

(ii) Each E_α is finite dimensional and consists of $C^\infty(G/K)$ functions

(iii) Each E_α is an irreducible representation subspace

(iv) If $\alpha \neq \beta$ then E_α and E_β are not isomorphic as representation subspaces.

The proof of the theorem is divided in seven steps.

Lemma A.2.6. *(i) and (ii) of Theorem A.2.5 holds.*

Proof. That E_α as defined in (A.2.3) is a representation subspace of $L^2(G/K)$ follows from $\lambda_g \circ T_h = T_h \circ \lambda_g$:

$$
\begin{aligned}
(\lambda_g T_h f)(x) &= (T_h f)(g^{-1}x) \\
&= \int_{G/K} h(g^{-1}x, y) f(y) \,\mathrm{d}y \\
&= \int_{G/K} h(x, gy) f(y) \,\mathrm{d}y \\
&= \int_{G/K} h(x, \eta) f(g^{-1}\eta) \,\mathrm{d}\eta = (T_h \lambda_g f)(x)\,.
\end{aligned}
$$

By Lemma A.1.22, T_h is a compact operator and, if h is real valued, it is also self-adjoint. Therefore, by spectral theorem,

$$L^2(G/K) = E_0 \oplus \left(\bigoplus_{\alpha \in \mathscr{A}} E_\alpha \right).$$

Where we used the fact that, for fixed $h \in L_K^2(G)$, (A.2.3) is an eigenvalue equation for T_h. Since G/K is a weakly symmetric space, T_h and T_k commutes for all $h, k \in L_K^2(G)$ and hence the decomposition (A.2.4) is independent of h.

Since T_h is compact, any of its eigenspaces (but eventually the one associated with eigenvalue zero) is finite dimensional. We need to prove that $E_0 = \{0\}$. Let us pick up φ_δ as in (A.1.23). Then, if $f \in E_0$, $T_{\varphi_\delta} f = 0$. Hence $f = \lim_{\delta \downarrow 0} T_{\varphi_\delta} f = 0$ (where we used the fact that T_{φ_δ} is an approximation of the identity in $L^2(G/K)$, Theorem A.1.18). This is sufficient to conclude that $E_0 = 0$.

Last, we prove the C^∞ regularity of functions in E_α. Using again Theorem A.1.18 together with (A.2.3) we have

$$f = \frac{1}{\alpha(\varphi_\delta)} T_{\varphi_\delta} f$$

Hence

$$\frac{\partial f(x)}{\partial x} = \frac{1}{\alpha(\varphi_\delta)} \int_{G/K} \frac{\partial \varphi_\delta(x, y)}{\partial x} f(y) \,\mathrm{d}y$$

and since $\varphi_\delta \in C^\infty(G/K \times G/K)$, we proved (ii). $\qquad\square$

Lemma A.2.7. *If $\{0\} \neq E \subset C(G/K)$ is any finite dimensional representation subspace, there is $p \in E^K$ with $p(\pi(e)) = 1$.*

Proof. Let $\delta_e : E \to \mathbb{C}$ be the evaluation map at $x = e$. This is well defined because $E \subset C(G/K)$ is a space of continuous functions. Since E is finite dimensional, every linear function on E can be uniquely represented as an inner product: there exists a unique $p_0 \in E$ such that $\forall f \in E$,

$$f(\pi(e)) \;=\; \int_{G/K} \overline{p_0(x)} f(x) \, \mathrm{d}x \,.$$

If $a \in K$ and $f \in E$ then using that the measure $\mathrm{d}x$ is invariant and the last equality we get

$$\int_{G/K} \overline{(\lambda_a p)(x)} f(x) \, \mathrm{d}x = \int_{G/K} \overline{p(a^{-1}x)} f(x) \mathrm{d}x$$
$$= \int_{G/K} \overline{p(x)} f(ax) \, \mathrm{d}x = f(a\pi(e)) = f(\pi(e)) \,.$$

Hence, since $p \in E$ is unique, this chain of equalities imply $\lambda_a p = p$ for all $a \in K$. Thus p is isotropic. As the action of G is transitive and $E \neq \{0\}$, there are functions $f \in E$ with $f(\pi(e)) \neq 0$ which implies $p_0 \neq 0$. Using $f = p_0$ we get

$$p_0(\pi(e)) \;=\; \int_{G/K} |p_0(x)|^2 \, \mathrm{d}x > 0 \,.$$

Choosing $p = \frac{1}{p_0(\pi(e))} p_0$ completes the proof. $\qquad\square$

Lemma A.2.8. *Each E_α^K is one-dimensional.*

Proof. From the previous Lemma A.2.7, there exists $p_\alpha \in E_\alpha^K$ with $p_\alpha(\pi(e)) = 1$. Let now $h_0 \in E_\alpha^K$ and set

$$h = h_0 - h_0(e)p_\alpha \,.$$

We start by noticing that $h(\pi(e)) = h_0(\pi(e)) - h_0(\pi(e))p_\alpha(\pi(e)) = 0$. As h is isotropic by definition, we can define (as we did in (A.1.18)-(A.1.19)) $H(x,y) = (\mathrm{Ext}\, h)(x,y) = h(\xi^{-1}y)$ where $\xi \in G$ is any element $\xi\pi(e) = x$.

From (A.2.3), $\forall f \in E_\alpha$

$$\alpha(H)f(x) = T_H f(x) = \int_{G/K} h(\xi^{-1}y)f(y) \, \mathrm{d}y$$

choosing $f = \overline{h}$ and $x = \pi(e)$ we get

$$0 = T_H \overline{h}(\pi(e)) = \int_{G/K} |h(y)|^2 \, \mathrm{d}y$$

and since h is continuous, the last equality implies $h = 0$. $\qquad\square$

Lemma A.2.9. *Each E_α is an irreducible representation subspace.*

Proof. If E_α was not irreducible, then we could decompose it as $E_\alpha = E_1 \oplus E_2$ with each E_i being a representation subspace containing an irreducible representation subspace. Then by Proposition A.2.4, $\dim E_\alpha^K = \dim E_1^K + \dim E_2^K \geqslant 2$. This contradicts Lemma A.2.8. $\qquad\square$

Lemma A.2.10. *Let $f_1, f_2 \in L^2(G/K)$. Then for each $\alpha \in \mathscr{A}$ there is a constant $c_\alpha(f_1, f_2)$ so that*

$$\int_{G/K} \int_{G/K} \overline{f_1(g^{-1}x)} f_2(g^{-1}y) \, \mathrm{d}g \, f(y) \, \mathrm{d}y = c_\alpha(f_1, f_2) f(x) \tag{A.2.5}$$

for any $f \in E_\alpha$.

Proof. Set $h(x, y) = \int_G f_1(g^{-1}x) f_2(g^{-1}y) \, \mathrm{d}g$. Using the fact that there is a unique Riemannian metric on G for which the submersion $\pi : G \to G/K$ is a Riemannian submersion, by Cauchy-Schwartz inequality and co-area formula,

$$\int_{G/K} |h(x, \pi(e))|^2 \, \mathrm{d}x = \int_{G/K} \left| \int_G \overline{f_1(g^{-1}x)} f_2(g^{-1}y) \right|^2 \, \mathrm{d}g \, \mathrm{d}x$$

$$\leqslant \int_{G/K} \int_G |f_1(g^{-1}x)|^2 \, \mathrm{d}g \int_G |f_2(\xi^{-1}y)|^2 \, \mathrm{d}\xi \, \mathrm{d}x$$

$$= \mu(G/K)\mu(K)^2 \|f_1\|_{L^2(G/K)}^2 \|f_2\|_{L^2(G/K)}^2 < +\infty$$

and using a similar argument $\int_{G/K} |h(\pi(e), y)|^2 \, \mathrm{d}y \leqslant \mu(G/K)\mu(K)^2 \|f_1\|_{L^2(G/K)}^2 \|f_2\|_{L^2(G/K)}^2 < +\infty$. To prove that $h \in L_K^2(G)$ it remains to see that for $\xi \in G$

$$h(\xi x, \xi y) = \int_G \overline{f_1(g^{-1}\xi x)} \, f_2(g^{-1}\xi y) \, \mathrm{d}g$$

$$= \int_G \overline{f_1(g^{-1}x)} \, f_2(g^{-1}y) \, \mathrm{d}g$$

$$= h(x, y) \,.$$

Thus $h \in L_K^2(G)$. If now $f \in E_\alpha$ we set $c_\alpha(f_1, f_2) := \alpha(h)$ and we get the thesis. □

Lemma A.2.11. *If $\alpha, \beta \in \mathscr{A}$ and $\alpha \neq \beta$ then E_α is not equivalent to E_β as a representation subspace.*

Proof. Let $\lambda_\alpha(g) := \lambda_g \restriction_{E_\alpha}$ and $\lambda_\beta(g) := \lambda_g \restriction_{E_\beta}$ be the induced representations on E_α and E_β. Let $\chi_\alpha(g) = \operatorname{tr} \lambda_\alpha(g)$ and $\chi_\beta(g) = \operatorname{tr} \lambda_\beta(g)$ be the corresponding characters. Suppose by contradiction that λ_α is equivalent to λ_β. By Lemma A.1.8, $\chi_\alpha(g) = \chi_\beta(g)$.

Choose an orthonormal basis $f_{\alpha,1}, \ldots, f_{\alpha,l}$ and $f_{\beta,1}, \ldots, f_{\beta,m}$ of E_α and E_β. In the basis $f_{\alpha,1}, \ldots, f_{\alpha,m}$ the matrix representing $\lambda_\alpha(g)$ is $[\lambda_\alpha(g)]_{ij} = \langle \lambda_\alpha(g)f_{\alpha,i}, f_{\alpha,j} \rangle$ and the trace is the sum of the diagonal elements of the matrix. Thus

$$\chi_\alpha(g) = \sum_{i=1}^{l} \langle \lambda_\alpha(g)f_{\alpha,i}, f_{\alpha,i} \rangle = \sum_{i=1}^{l} \int_{G/K} \overline{f_{\alpha,i}(g^{-1}x)} \, f_{\alpha,i}(x) \, \mathrm{d}x$$

and likewise

$$\chi_\beta(g) = \sum_{j=1}^{m} \int_{G/K} \overline{f_{\beta,j}(g^{-1}y)} \, f_{\beta,j}(y) \, \mathrm{d}y \,.$$

Using these relations and interchanging the order of integration we get

$$\int_G \overline{\chi_\alpha(g)} \chi_\beta(g) \, \mathrm{d}g$$

$$= \sum_{i,j} \int_{G/K} \left(\int_{G/K} \int_G f_{\alpha,i}(g^{-1}x) \overline{f_{\beta,j}(g^{-1}y)} \, \mathrm{d}g \, f_{\beta,j}(y) \, \mathrm{d}y \right) \overline{f_{\alpha,i}(x)} \, \mathrm{d}x$$

$$= \sum_{i,j} \overline{c_\beta(f_{\alpha,i}, f_{\beta,j})} \int_{G/K} f_{\beta,j}(x) \overline{f_{\alpha,i}(x)} \, \mathrm{d}x = 0$$

where in the last step we used the orthogonality of E_α and E_β. But if E_α and E_β are isomorphic, then $\chi_\alpha = \chi_\beta$ and this leads to the contradiction $0 = \int_G \overline{\chi_\alpha(g)} \chi_\beta(g) \, \mathrm{d}g = \int_G |\chi_\alpha(g)|^2 \, \mathrm{d}g > 0$. $\qquad\square$

Lemma A.2.12. *If $\{0\} \neq E \subset L^2(G/K)$ is a finite dimensional irreducible representation space, then $E = E_{\alpha_0}$ for some α_0.*

Proof. Let $P_\alpha : L^2(G/K) \to E_\alpha$ be the orthogonal projection of $L^2(G/K)$ onto E_α. Then both E_α and $E_\alpha^\perp$ are invariant under the action of G and P_α is an intertwining map. If $P_\alpha E = \{0\}$ for all α, then $E = \{0\}$ as $L^2(G/K) = \bigoplus_{\alpha \in \mathscr{A}} E_\alpha$. Thus for some α_0, $P_{\alpha_0} E_{\alpha_0} \neq \{0\}$. The map $P_{\alpha_0} \restriction_E$: $E \to E_{\alpha_0}$ is a nonzero intertwining map, thus by Shur's lemma (Lemma A.1.7), $P_{\alpha_0} \restriction_E$: $E \to E_{\alpha_0}$ is an isomorphism. Thus E is isomorphic to E_{α_0} as representation subspace. If $\alpha \neq \alpha_0$ then, by the last step, E_α and E_{α_0} are not isomorphic as representation subspaces and thus Shur's lemma implies $P_\alpha \restriction_E$: $E \to E_\alpha$ is the zero map for $\alpha \neq \alpha_0$. This implies $E \subset E_{\alpha_0}$. And since E is a nonzero representation subspace of E_{α_0} and since E_{α_0} is irreducible, then $E = E_{\alpha_0}$. $\qquad\square$

Note that, by definition (A.2.3), since for a fixed $h \in L_K^2(G)$ the operator T_h is compact (Lemma A.1.22), the cardinality of $\mathscr{A}$ is at most $\aleph_0$ (the cardinality of $\mathbb{N}$). Since $L^2(G/K)$ is an infinite dimensional space, one of the consequences of Theorem A.2.5 is that the cardinality of $\mathscr{A}$ is exactly $\aleph_0$. If this was not true, then from (A.2.4), we would obtain $\dim L^2(G/K) < \infty$ which is absurd.

Bibliography

[1] M. ABRAMOWITZ AND I. A. STEGUN, *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, vol. 55 of National Bureau of Standards Applied Mathematics Series, For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 1964.

[2] A. AGRACHEV, U. BOSCAIN, AND M. SIGALOTTI, *A Gauss-Bonnet-like formula on two-dimensional almost-Riemannian manifolds*, Discrete Contin. Dyn. Syst., 20 (2008), pp. 801–822.

[3] S. ALBEVERIO, F. GESZTESY, R. HØ EGH-KROHN, AND L. STREIT, *Charged particles with short range interactions*, Ann. Inst. H. Poincaré Sect. A (N.S.), 38 (1983), pp. 263–293.

[4] S. ALBEVERIO, F. GESZTESY, R. HØEGH-KROHN, AND H. HOLDEN, *Solvable Models in Quantum Mechanics*, Texts and Monographs in Physics, Springer-Verlag, New York, 1988.

[5] A. ALONSO AND B. SIMON, *The Birman-Kreĭn-Vishik theory of selfadjoint extensions of semibounded operators*, J. Operator Theory, 4 (1980), pp. 251–270.

[6] T. ANDO AND K. NISHIO, *Positive selfadjoint extensions of positive symmetric operators*, Tôhoku Math. J. (2), 22 (1970), pp. 65–75.

[7] M. ARAI, *On Essential Self-Adjointness of Dirac Operators*, Publ. Res. Inst. Math. Sci., 242 (1975), pp. 10–21.

[8] ——, *On essential selfadjointness, distinguished selfadjoint extension and essential spectrum of Dirac operators with matrix valued potentials*, Publ. Res. Inst. Math. Sci., 19 (1983), pp. 33–57.

[9] M. ARAI AND O. YAMADA, *Essential selfadjointness and invariance of the essential spectrum for Dirac operators*, Publ. Res. Inst. Math. Sci., 18 (1982), pp. 973–985.

[10] N. ARRIZABALAGA, *Distinguished self-adjoint extensions of Dirac operators via Hardy-Dirac inequalities*, J. Math. Phys., 52 (2011), pp. 092301, 14.

[11] N. ARRIZABALAGA, J. DUOANDIKOETXEA, AND L. VEGA, *Self-adjoint extensions of Dirac operators with Coulomb type singularity*, J. Math. Phys., 54 (2013), pp. 041504, 20.

[12] V. B. BERESTETSKII, E. M. LIFSHITZ, AND L. P. PITAEVSKII, *Course of theoretical physics, Vol. 4. Quantum Electrodynamics*, Pergamon Press, Oxford-New York-Toronto, Ont., second ed., 1982. Translated from the Russian by J. B. Sykes and J. S.Bell.

[13] A. BERTHIER AND V. GEORGESCU, *On the point spectrum of Dirac operators*, J. Funct. Anal., 71 (1987), pp. 309–338.

[14] H. A. BETHE AND E. E. SLAPETER, *Quantum Mechanics of One- and Two-Electron Atoms*, Springer-Verlag Berlin Heidelberg, 1957.

[15] M. V. BIRMAN, *On the theory of self-adjoint extensions of positive definite operators*, Mat. Sb. N.S., 38(80) (1956), pp. 431–450.

[16] U. BOSCAIN AND C. LAURENT, *The Laplace-Beltrami operator in almost-Riemannian geometry*, Ann. Inst. Fourier (Grenoble), 63 (2013), pp. 1739–1770.

[17] U. BOSCAIN AND D. PRANDI, *Self-adjoint extensions and stochastic completeness of the laplace–beltrami operator on conic and anticonic surfaces*, Journal of Differential Equations, 260 (2016), pp. 3234–3269.

[18] M. BRAVERMAN, O. MILATOVICH, AND M. SHUBIN, *Essential selfadjointness of Schrödinger-type operators on manifolds*, Uspekhi Mat. Nauk, 57 (2002), pp. 3–58.

[19] L. BRUNEAU, J. DEREZIŃSKI, AND V. GEORGESCU, *Homogeneous Schrödinger operators on half-line*, Ann. Henri Poincaré, 12 (2011), pp. 547–590.

[20] ——, *Homogeneous Schrödinger operators on half-line*, Ann. Henri Poincaré, 12 (2011), pp. 547–590.

[21] W. BULLA AND F. GESZTESY, *Deficiency indices and singular boundary conditions in quantum mechanics*, J. Math. Phys., 26 (1985), pp. 2520–2528.

[22] C. BURNAP, H. BRYSK, AND P. F. ZWEIFEL, *Dirac Hamiltonian for strong Coulomb fields*, Il Nuovo Cimento B (1971-1996), 64 (1981), pp. 407–419.

[23] M. CALÇADA, J. T. LUNARDI, L. A. MANZONI, W. MONTEIRO, AND M. PEREIRA, *A distributional approach for the one-dimensional hydrogen atom*, Frontiers in Physics, 7 (2019), p. 101.

[24] O. CALIN AND D.-C. CHANG, *Sub-Riemannian geometry*, vol. 126 of Encyclopedia of Mathematics and its Applications, Cambridge University Press, Cambridge, 2009. General theory and examples.

[25] J. W. CALKIN, *Symmetric transformations in Hilbert space*, Duke Math. J., 7 (1940), pp. 504–508.

[26] B. CASSANO AND F. PIZZICHILLO, *Self-adjoint extensions for the dirac operator with coulomb-type spherically symmetric potentials*, Letters in Mathematical Physics, 108 (2018), pp. 2635–2667.

[27] ——, *Boundary triples for the dirac operator with coulomb-type spherically symmetric perturbations*, Journal of Mathematical Physics, 60 (2019), p. 041502.

[28] P. R. CHERNOFF, *Schrödinger and Dirac operators with singular potentials and hyperbolic equations*, Pacific J. Math., 72 (1977), pp. 361–382.

[29] E. A. CODDINGTON AND H. S. V. DE SNOO, *Positive selfadjoint extensions of positive symmetric subspaces*, Math. Z., 159 (1978), pp. 203–214.

[30] F. COOPER, A. KHARE, R. MUSTO, AND A. WIPF, *Supersymmetry and the Dirac equation*, Annals of Physics, 187 (1988), pp. 1–28.

[31] M. CORREGGI, G. DELL'ANTONIO, D. FINCO, A. MICHELANGELI, AND A. TETA, *Stability for a system of N fermions plus a different particle with zero-range interactions*, Rev. Math. Phys., 24 (2012), pp. 1250017, 32.

[32] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon, *Schrödinger operators with application to quantum mechanics and global geometry*, Texts and Monographs in Physics, Springer-Verlag, Berlin, study ed., 1987.

[33] C. G. Darwin, *The wave equations of the electron*, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 118 (1928), pp. 654–680.

[34] G. Dell'Antonio and A. Michelangeli, *Schrödinger operators on half-line with shrinking potentials at the origin*, Asymptot. Anal., 97 (2016), pp. 113–138.

[35] J. Dereziński and S. Richard, *On Schrödinger operators with inverse square potentials on the half-line*, Ann. Henri Poincaré, 18 (2017), pp. 869–928.

[36] ———, *On radial Schrödinger operators with a Coulomb potential*, arXiv:1712.04068 (2017).

[37] V. A. Derkach and M. M. Malamud, *Generalized resolvents and the boundary value problems for Hermitian operators with gaps*, J. Funct. Anal., 95 (1991), pp. 1–95.

[38] N. Dunford and J. T. Schwartz, *Linear operators. Part II: Spectral theory. Self adjoint operators in Hilbert space*, With the assistance of William G. Bade and Robert G. Bartle, Interscience Publishers John Wiley & Sons New York-London, 1963.

[39] M. Erceg and A. Michelangeli, *On Contact Interactions Realised as Friedrichs Systems*, Complex Analysis and Operator Theory, (2018).

[40] M. Esteban, M. Lewin, and É. Séré, *Domains for dirac–coulomb min-max levels*, Revista Matemática Iberoamericana, 35 (2019), pp. 877–924.

[41] M. J. Esteban and M. Loss, *Self-adjointness for Dirac operators via Hardy-Dirac inequalities*, J. Math. Phys., 48 (2007), pp. 112107, 8.

[42] W. D. Evans, *On the unique self-adjoint extension of the Dirac operator and the existence of the Green matrix*, Proc. London Math. Soc. (3), 20 (1970), pp. 537–557.

[43] S. Fluügge and H. Marschall, *Rechenmethoden der Quantentheorie*, Springer-Verlag Berlin Heidelberg, Oxford, 1952.

[44] V. Franceschi, D. Prandi, and L. Rizzi, *On the essential self-adjointness of singular sub-Laplacians*, arXiv:1708.09626 (2017).

[45] K. Friedrichs, *Spektraltheorie halbbeschränkter Operatoren und Anwendung auf die Spektralzerlegung von Differentialoperatoren*, Math. Ann., 109 (1934), pp. 465–487.

[46] M. P. Gaffney, *A special Stokes's theorem for complete Riemannian manifolds*, Ann. of Math. (2), 60 (1954), pp. 140–145.

[47] M. Gallone, *Self-Adjoint Extensions of Dirac Operator with Coulomb Potential*, in Advances in Quantum Mechanics, G. Dell'Antonio and A. Michelangeli, eds., vol. 18 of INdAM-Springer series, Springer International Publishing, pp. 169–186.

[48] M. Gallone and A. Michelangeli, *Discrete spectra for critical Dirac-Coulomb Hamiltonians*, J. Math. Phys., 59 (2018), pp. 062108, 19.

[49] M. Gallone and A. Michelangeli, *Hydrogenoid spectra with central perturbations*, 2018.

[50] M. Gallone and A. Michelangeli, *Self-adjoint realisations of the Dirac-Coulomb Hamiltonian for heavy nuclei*, Analysis and Mathematical Physics, (2018).

[51] M. Gallone, A. Michelangeli, and A. Ottolini, *Kreĭn-Višik-Birman self-adjoint extension theory revisited*, SISSA preprint 25/2017/MATE (2017).

[52] M. Gallone, A. Michelangeli, and E. Pozzoli, *On geometric quantum confinement in grushin-type manifolds*, 2018.

[53] V. Georgescu and M. Măntoiu, *On the spectral theory of singular Dirac type Hamiltonians*, J. Operator Theory, 46 (2001), pp. 289–321.

[54] F. Gesztesy and M. Zinchenko, *On spectral theory for Schrödinger operators with strongly singular potentials*, Math. Nachr., 279 (2006), pp. 1041–1082.

[55] D. M. Gitman, I. V. Tyutin, and B. L. Voronov, *Self-adjoint extensions in quantum mechanics*, vol. 62 of Progress in Mathematical Physics, Birkhäuser/Springer, New York, 2012. General theory and applications to Schrödinger and Dirac equations with singular potentials.

[56] M. L. Gorbačuk and V. A. Mihaĭlec, *Semibounded selfadjoint extensions of symmetric operators*, Dokl. Akad. Nauk SSSR, 226 (1976), pp. 765–767.

[57] H. Grosse, *On the level order for Dirac operators*, Phys. Lett. B, 197 (1987), pp. 413–417.

[58] G. Grubb, *A characterization of the non-local boundary value problems associated with an elliptic operator*, Ann. Scuola Norm. Sup. Pisa (3), 22 (1968), pp. 425–513.

[59] ——, *Properties of normal boundary problems for elliptic even-order systems*, Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4), 1 (1974), pp. 1–61 (1975).

[60] ——, *Distributions and operators*, vol. 252 of Graduate Texts in Mathematics, Springer, New York, 2009.

[61] K. E. Gustafson and P. A. Rejto, *Some essentially self-adjoint Dirac operators with spherically symmetric potentials*, Israel J. Math., 14 (1973), pp. 63–75.

[62] B. C. Hall, *Quantum theory for mathematicians*, vol. 267 of Graduate Texts in Mathematics, Springer, New York, 2013.

[63] B. C. Hall, *Lie Groups, Lie Algebras, and Representations*, Springer International Publishing, 2015.

[64] H. Hogreve, *The overcritical Dirac-Coulomb operator*, J. Phys. A, 46 (2013), pp. 025301, 22.

[65] L. Hostler, *Runge-Lenz Vector and the Coulomb Green's Function*, J. Math. Phys., 8 (1967), pp. 642–646.

[66] R. V. Kadison, *Isometries of operator algebras*, The Annals of Mathematics, 54 (1951), p. 325.

[67] R. V. Kadison, *Some notes on noncommutative analysis*, in Analysis at Urbana, Vol. II (Urbana, IL, 1986–1987), vol. 138 of London Math. Soc. Lecture Note Ser., Cambridge Univ. Press, Cambridge, 1989, pp. 243–257.

[68] H. Kalf, U.-W. Schmincke, J. Walter, and R. Wüst, *On the spectral theory of Schrödinger and Dirac operators with strongly singular potentials*, (1975), pp. 182–226. Lecture Notes in Math., Vol. 448.

[69] T. Kato, *Fundamental properties of hamiltonian operators of schrödinger type*, Transactions of the American Mathematical Society, 70 (1951), pp. 195–195.

[70] T. Kato, *Holomorphic families of Dirac operators*, Math. Z., 183 (1983), pp. 399–406.

[71] ——, *Perturbation theory for linear operators*, Classics in Mathematics, Springer-Verlag, Berlin, 1995. Reprint of the 1980 edition.

[72] M. KLAUS AND R. WÜST, *Characterization and uniqueness of distinguished selfadjoint extensions of Dirac operators*, Comm. Math. Phys., 64 (1978/79), pp. 171–176.

[73] V. KOSTRYKIN AND R. SCHRADER, *Laplacians on metric graphs: eigenvalues, resolvents and semigroups*, in Quantum graphs and their applications, vol. 415 of Contemp. Math., Amer. Math. Soc., Providence, RI, 2006, pp. 201–225.

[74] M. G. KREĬN, *The theory of self-adjoint extensions of semi-bounded Hermitian transformations and its applications. I*, Rec. Math. [Mat. Sbornik] N.S., 20(62) (1947), pp. 431–495.

[75] M. G. KREĬN AND M. A. KRASNOSEL′SKIĬ, *Fundamental theorems on the extension of Hermitian operators and certain of their applications to the theory of orthogonal polynomials and the problem of moments*, Uspehi Matem. Nauk (N. S.), 2 (1947), pp. 60–106.

[76] J. J. LANDGREN AND P. A. REJTO, *An application of the maximum principle to the study of essential selfadjointness of Dirac operators. I*, J. Math. Phys., 20 (1979), pp. 2204–2211.

[77] ——, *On a theorem of Jörgens and Chernoff concerning essential selfadjointness of Dirac operators*, J. Reine Angew. Math., 322 (1981), pp. 1–14.

[78] J. J. LANDGREN, P. A. REJTO, AND M. KLAUS, *An application of the maximum principle to the study of essential self-adjointness of Dirac operators. II*, Journal of Mathematical Physics, 21 (1980), pp. 1210–1217.

[79] J. LEE, *Introduction to Smooth Manifolds*, Graduate Texts in Mathematics, Springer, 2003.

[80] E. H. LIEB AND M. LOSS, *Analysis*, vol. 14 of Graduate Studies in Mathematics, American Mathematical Society, Providence, RI, second ed., 2001.

[81] R. LOUDON, *One-dimensional Hydrogen atom*, Proceedings of the Royal Society A, 472 (2016).

[82] A. M. MEL′NIKOV AND R. A. MINLOS, *On the pointlike interaction of three different particles*, in Many-particle Hamiltonians: spectra and scattering, vol. 5 of Adv. Soviet Math., Amer. Math. Soc., Providence, RI, 1991, pp. 99–112.

[83] ——, *Point interaction of three different particles*, Vestnik Moskov. Univ. Ser. I Mat. Mekh., 3 (1991), pp. 3–6, 110.

[84] A. MICHELANGELI AND A. OTTOLINI, *On point interactions realised as Ter-Martirosyan-Skornyakov Hamiltonians*, Rep. Math. Phys., 79 (2017), pp. 215–260.

[85] R. A. MINLOS, *On the point interaction of three particles*, in Applications of selfadjoint extensions in quantum physics (Dubna, 1987), vol. 324 of Lecture Notes in Phys., Springer, Berlin, 1989, pp. 138–145.

[86] ——, *A system of three pointwise interacting quantum particles*, Uspekhi Mat. Nauk, 69 (2014), pp. 145–172.

[87] R. A. MINLOS AND L. D. FADDEEV, *Comment on the problem of three particles with point interactions*, Soviet Physics JETP, 14 (1962), pp. 1315–1316.

[88] ——, *On the point interaction for a three-particle system in quantum mechanics*, Soviet Physics Dokl., 6 (1962), pp. 1072–1074.

[89] G. NENCIU, *Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms*, Comm. Math. Phys., 48 (1976), pp. 235–247.

[90] G. NENCIU AND I. NENCIU, *On confining potentials and essential self-adjointness for Schrödinger operators on bounded domains in $\mathbb{R}^n$*, Ann. Henri Poincaré, 10 (2009), pp. 377–394.

[91] H. PANAHI AND Z. BAKHSHI, *Dirac Equation and Ground State of Solvable Potentials: Supersymmetry Method*, International Journal of Theoretical Physics, 50 (2011), pp. 2811–2818.

[92] E. POZZOLI, *Models of quantum confinement and perturbative methods for point interactions*, Master Thesis (2018).

[93] D. PRANDI, L. RIZZI, AND M. SERI, *Quantum confinement of non-complete Riemannian manifolds*, arXiv:1609.01724 (2016).

[94] V. PROKAJ AND Z. SEBESTYÉN, *On extremal positive operator extensions*, Acta Sci. Math. (Szeged), 62 (1996), pp. 485–491.

[95] M. REED AND B. SIMON, *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness*, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975.

[96] ——, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1978.

[97] P. A. REJTO, *Some essentially self-adjoint one-electron Dirac operators. (With appendix.)*, Israel J. Math., 9 (1971), pp. 144–171.

[98] F. RELLICH, *Die zulässigen Randbedingungen bei den singulären Eigenwertproblemen der mathematischen Physik. (Gewöhnliche Differentialgleichungen zweiter Ordnung.)*, Math. Z., 49 (1944), pp. 702–723.

[99] F. RELLICH, K. JÖRGENS, AND U. G. M. INSTITUT, *Eigenwerttheorie partieller Differentialgleichungen: Vorlesung, gehalten an der Universität Göttingen*, Eigenwerttheorie partieller Differentialgleichungen, Mathematisches Institut der Universität Göttingen, 1953.

[100] B. W. ROOS AND W. C. SANGREN, *Spectral theory of dirac's radial relativistic wave equation*, Journal of Mathematical Physics, 3 (1962), pp. 882–890.

[101] ——, *Spectral theory of dirac's radial relativistic wave equation*, Journal of Mathematical Physics, 3 (1962), pp. 882–890.

[102] U.-W. SCHMINCKE, *Distinguished selfadjoint extensions of Dirac operators*, Math. Z., 129 (1972), pp. 335–349.

[103] ——, *Essential selfadjointness of Dirac operators with a strongly singular potential*, Math. Z., 126 (1972), pp. 71–81.

[104] K. SCHMÜDGEN, *Unbounded self-adjoint operators on Hilbert space*, vol. 265 of Graduate Texts in Mathematics, Springer, Dordrecht, 2012.

[105] E. SCHRÖDINGER, *Quantisierung als Eigenwertproblem (Erste Mitteilung). (German) [Quantization as an eigenvalue problem (First report)]*, 384 (1926), pp. 361–376.

[106] Z. SEBESTYÉN AND J. STOCHEL, *Restrictions of positive selfadjoint operators*, Acta Sci. Math. (Szeged), 55 (1991), pp. 149–154.

[107] ——, *Characterizations of positive selfadjoint extensions*, Proc. Amer. Math. Soc., 135 (2007), pp. 1389–1397 (electronic).

[108] M. H. STONE, *Linear transformations in Hilbert space*, vol. 15 of American Mathematical Society Colloquium Publications, American Mathematical Society, Providence, RI, 1932.

[109] C. V. SUKUMAR, *Supersymmetry and the Dirac equation for a central Coulomb field*, J. Phys. A, 18 (1985), pp. L697–L701.

[110] M. TAKESAKI, *Tomita's theory of modular Hilbert algebras and its applications*, Lecture Notes in Mathematics, Vol. 128, Springer-Verlag, Berlin-New York, 1970.

[111] B. THALLER, *The Dirac equation*, Texts and Monographs in Physics, Springer-Verlag, Berlin, 1992.

[112] M. I. VIŠIK, *On general boundary problems for elliptic differential equations*, Trudy Moskov. Mat. Obšč., 1 (1952), pp. 187–246.

[113] J. VON NEUMANN, *Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren*, Math. Ann., 102 (1930), pp. 49–131.

[114] B. L. VORONOV, D. M. GITMAN, AND I. V. TYUTIN, *The Dirac Hamiltonian with a superstrong Coulomb field*, Teoret. Mat. Fiz., 150 (2007), pp. 41–84.

[115] A. D. WARD, *The essential self-adjointness of Schrödinger operators on domains with non-empty boundary*, Manuscripta Math., 150 (2016), pp. 357–370.

[116] W. WASOW, *Asymptotic expansions for ordinary differential equations*, Dover Publications, Inc., New York, 1987. Reprint of the 1976 edition.

[117] J. WEIDMANN, *Oszillationsmethoden für Systeme gewöhnlicher Differentialgleichungen*, Math. Z., 119 (1971), pp. 349–373.

[118] ——, *Linear operators in Hilbert spaces*, vol. 68 of Graduate Texts in Mathematics, Springer-Verlag, New York-Berlin, 1980. Translated from the German by Joseph Szücs.

[119] ——, *Spectral theory of ordinary differential operators*, vol. 1258 of Lecture Notes in Mathematics, Springer-Verlag, Berlin, 1987.

[120] H. WEYL, *über gewöhnliche differentialgleichungen mit singularitäten und die zugehörigen entwicklungen willkürlicher funktionen*, Mathematische Annalen, 68 (1910), pp. 220–269.

[121] E. P. WIGNER AND U. FANO, *Group theory and its application to the quantum mechanics of atomic spectra*, American Journal of Physics, 28 (1960), pp. 408–409.

[122] R. WÜST, *Distinguished self-adjoint extensions of Dirac operators constructed by means of cut-off potentials*, Math. Z., 141 (1975), pp. 93–98.

[123] ——, *Dirac operations with strongly singular potentials. Distinguished self-adjoint extensions constructed with a spectral gap theorem and cut-off potentials*, Math. Z., 152 (1977), pp. 259–271.

[124] J. XIA, *On the contribution of the Coulomb singularity of arbitrary charge to the Dirac Hamiltonian*, Trans. Amer. Math. Soc., 351 (1999), pp. 1989–2023.

[125] K. ZHU, *Operator Theory in Function Spaces*, Mathematical surveys and monographs, American Mathematical Soc.

[126] J. ZORBAS, *Perturbation of self-adjoint operators by Dirac distributions*, J. Math. Phys., 21 (1980), pp. 840–847.