Spectra of self-adjoint extensions and applications to solvable Schrödinger operators

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Abstract

We give a self-contained presentation of the theory of self-adjoint extensions using the technique of boundary triples. A description of the spectra of self-adjoint extensions in terms of the corresponding Krein maps (Weyl functions) is given. Applications include quantum graphs, point interactions, hybrid spaces, singular perturbations.

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0   Introduction

In recent two decades, the field of applications of explicitly solvable models of quantum mechanics based on the operator extension technique has been expanded considerably. New scopes are presented e.g. in the Appendix by P. Exner [56] to the second edition of the monograph [6], in the monograph by S. Albeverio and P. Kurasov [9], and in the topical issue of the Journal of Physics A [44]. A review of papers dealing with the theory of Aharonov–Bohm effects from the point of view of the operator methods is contained in [65, 103]; new methods of analyzing singular perturbations supported by sets with non-trivial geometry are reviewed in [58]. In addition, one should mention the use of such models in the quantum field theory [70, 80], including string theory [86], quantum gravity [123], and quantum cosmology (see S. P. Novikov's comment in [74] to results from [73]). Here the two-dimensional δ-like potential, which is a point supported perturbation, is of considerable interest because in this case the Dirac

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δ-function has the same dimension as the Laplacian, and this property leads to an effective non-perturbative renormalization procedure removing the ultraviolet divergence [40, 82, 83]. Another peculiarity of the two-dimensional case – so-called dimensional transmutation – was observed in [39, 41]. The operator extension technique allows to build "toy models" which help better understanding some phenomena in various fields of mathematics and theoretical physics; as typical examples we mention here the spectral theory of automorphic functions [32] or renormalization group theory [3]. This technique is applicable not only to self-adjoint operators, it can be used, e.g. in investigating dissipative and accumulative operators as well [85].

Very important applications of the operator extension theory have been found recently in the physics of mesoscopic systems like heterostructures [72], quantum graphs [90, 91, 93, 106] and circuits [1], quantum wells, dots, and wires [81]. It should be stressed that in this case, the corresponding results are not only of qualitative character, but allow to give a good quantitative explanation of experimental data (see e.g. [28, 79]) or explain some discrepancy between experimental data and standard theories [29].

Among the most popular ways of using singular perturbations in the physics literature one should mention first of all various renormalization procedures including the Green function renormalization and cut-off potentials in the position or momentum representations (see [6] and an informative citation list in [110]). Berezin and Faddeev [20] were first who showed that the renormalization approach to singular perturbations is equivalent to searching for self-adjoint extensions of a symmetric operator related to the unperturbed operator in question. At the same time, the mathematical theory of self-adjoint extensions is reduced as a rule to the classical von Neumann description through unitary operators in deficiency spaces, which makes its practical use rather difficult. In many cases self-adjoint operators arise when one introduces some boundary conditions for a differential expression (like boundary conditions for the Laplacian in a domain), and it would be useful to analyze the operators in terms of boundary conditions directly. Such an approach is common in the physics literature [15, 45]. In the framework of the abstract mathematical theory of self-adjoint (or, more generally, dissipative) extensions this approach is widely used in the differential operator theory (see e.g., [53, 71, 75] and the historical as well as the bibliographical comments therein). Moreover, there is a series of quantum mechanics problems related to the influence of topological boundaries, and in this case the above approach is the most adequate [13].

On the other hand, Berezin and Faddeev pointed out that the standard expressions for the Green functions of singularly perturbed Hamiltonians obtained by the renormalization procedure can be easy derived from the so-called Krein resolvent formula [20]. In the framework of the theory of explicitly solvable mod-

els with an internal structure, an elegant way to get the Krein resolvent formula with the help of abstract boundary conditions has been proposed by Pavlov [111] (see also [2]), which was applied to the study of numerous applications, see e. g. [61, 94, 99, 102, 112]. A machinery of self-adjoint extensions using abstract boundary condisitons is presented in a rather detailed form in the monograph [71], but only very particular questions of the spectral theory are adressed. A systematic theory of self-adjoint extensions in terms of boundary conditions, including the spectral analysis, was developed by Derkach and Malamud, who found, in particular, a nice relationship between the parameters of self-adjoint extensions and the Krein resolvent formula, and performed the spectral analysis in terms of the Weyl functions; we refer to the paper [49] summarizing this machinery and containing an extensive bibliography.

Nevertheless, one has to admit that the spectral analysis of self-adjoint extensions in such terms is a rarely used tool in the analysis of quantum-mechanical Hamiltonians, especially for operators with infinite deficiency indices. On the other hand, the authors' experience show that the application of the Krein resolvent formula in combination with the boundary values for self-adjoint extensions can advance in solutions of some problems related to the applications of singular perturbations [30, 34, 35]. Therefore, it is useful to give a self-contained exposition of the abstract technique of boundary value problems and to analyze some models of mathematical physics using this machinery. This is the first aim of the present paper.

Using the Krein resolvent formula, it is possible often to reduce the spectral problem for the considered perturbed operator to a problem of finding the kernel of an analytic family of operators – so-called Krein $\mathscr{Q}$-function – with more simple structure in comparison with the operator in question. Therefore, it would be useful to find relations between various parts of the spectrum of the considered operators and the corresponding parts of the spectrum of $\mathscr{Q}$-functions. The second aim of the paper is to describe these relations in a form suitable for applications. Using the corresponding results, we obtain, in particular, new properties of the spectra of equilateral quantum graphs and arrays of quantum dots. Of course, we believe that the technique presented here can be used to analyze much more general systems. It is worth noting that this problem was considered in [24], but the main results were obtained in a form which is difficult to use for our applications.

In Section 1 we describe the machinery of boundary triples and their applications to self-adjoint extensions. The most results in this section are not new (we give the corresponding references in the text), but we do not know any work where this theory was presented with complete proofs, hence we decided to do it here. We also relate the technique of boundary triples with the so-called Krein $\mathscr{Q}$-functions and Γ-fields. Some of our definitions are slightly different from

the commonly used ones (although we show later that the both are equivalent); this is motivated by applied needs. We conclude the section by several examples showing that the machinery of boundary triples include the well known situations like singular perturbations, point perturbation, hybrid spaces. Section 2 is a summary of a necessary information about the spectra and spectral measures of self-adjoint operators. In Section 3 we provide the spectral analysis of self-adjoint extensions with the help of the Krein $\mathscr{Q}$-functions. In particular, we analyze the discrete and essential spectra, and carry out a complete spectral analysis for a special class of $\mathscr{Q}$-functions, which includes the recently introduced scalar-type functions [5]; these results are new. Using these results we analyze two classes of quantum-mechanical models: equilateral quantum graphs and arrays of quantum dots, where we perform the complete dimension reduction and describe the spectra of continuous models completely in terms of the associated tight-binding Hamiltonians. Section 4 is devoted to the study of isolated eigenvalues of self-adjoint extensions and generalizes previously known results to the case of operators with infinite deficiency indices.

The second named author, Vladimir Geyler, passed away on April 2, 2007, several days after the completion and the submission of the manuscript. His untimely death has become a great loss for us.

1 Abstract self-adjoint boundary value problems

In this section we describe the theory of self-adjoint extensions using abstract boundary conditions. Some theorems here are not new, but the existing presentations are spread through the literature, so we decided to provide here the key ideas with complete proofs.

1.1 Linear relations

Here we recall some basic facts on linear relations. For a more detailed discussion we refer to [12]. Let $\mathscr{G}$ be a Hilbert space. Any linear subspace of $\mathscr{G} \oplus \mathscr{G}$ will be called a *linear relation* in $\mathscr{G}$. For a linear relation Λ in $\mathscr{G}$ the sets

$$\operatorname{dom}\Lambda := \{x \in \mathscr{G} : \exists y \in \mathscr{G} \text{ with } (x,y) \in \Lambda\},$$
$$\operatorname{ran}\Lambda := \{x \in \mathscr{G} : \exists y \in \mathscr{G} \text{ with } (y,x) \in \Lambda\},$$
$$\ker\Lambda := \{x \in \mathscr{G} : (x,0) \in \Lambda\}$$

will be called the *domain*, the *range*, and the *kernel* of Λ, respectively. The linear relations

$$\Lambda^{-1} = \{(x,y) \in \mathscr{G} \oplus \mathscr{G} : (y,x) \in \Lambda\},$$
$$\Lambda^* = \{(x_1,x_2) \in \mathscr{G} \oplus \mathscr{G} : \langle x_1|y_2 \rangle = \langle x_2|y_1 \rangle \quad \forall (y_1,y_2) \in \Lambda\}$$

are called *inverse* and *adjoint* to Λ, respectively. For $\alpha \in \mathbb{C}$ we put

$$\alpha\Lambda = \{(x,\alpha y) : (x,y) \in \Lambda\}.$$

For two linear relations $\Lambda', \Lambda'' \subset \mathscr{G} \oplus \mathscr{G}$ one can define their *sum*

$$\Lambda' + \Lambda'' = \{(x,y'+y'') : (x,y') \in \Lambda', (x,y'') \in \Lambda''\};$$

clearly, one has $\mathrm{dom}(\Lambda' + \Lambda'') = \mathrm{dom}\,\Lambda' \cap \mathrm{dom}\,\Lambda''$. The graph of any linear operator L with domain in $\mathscr{G}$ is a linear relation, which we denote by $\mathrm{gr}\,L$. Clearly, if L is invertible, then $\mathrm{gr}\,L^{-1} = (\mathrm{gr}\,L)^{-1}$. For arbitrary linear operators L', L'' one has $\mathrm{gr}\,(\alpha L) = \alpha\,\mathrm{gr}\,L$ and $\mathrm{gr}\,L' + \mathrm{gr}\,L'' = \mathrm{gr}\,(L' + L'')$. Therefore, the set of linear operators has a natural "linear" imbedding into the set of linear relations. Moreover, if L is a densely defined closable operator in $\mathscr{G}$, then $\mathrm{gr}\,L^* = (\mathrm{gr}\,L)^*$, hence, this imbedding commutes with the star-operation.

In what follows we consider mostly only closed linear relations, i.e. which are closed linear subspaces in $\mathscr{G} \oplus \mathscr{G}$. Clearly, this generalizes the notion of a closed operator. Similarly to operators, one introduces the notion of the *resolvent set* $\mathrm{res}\,\Lambda$ of a linear relation Λ. By definition, $\lambda \in \mathrm{res}\,\Lambda$ if $(\Lambda - \lambda I)^{-1}$ is the graph of a certain everywhere defined bounded linear operator (here $I \equiv \mathrm{gr}\,\mathrm{id}_{\mathscr{G}} = \{(x,x) : x \in \mathscr{G}\}$); this operator will be also denoted as $(\Lambda - \lambda I)^{-1}$. Due to the closed graph theorem, the condition $\lambda \in \mathrm{res}\,\Lambda$ exactly means that Λ is closed, $\ker(\Lambda - \lambda I) = 0$, and $\mathrm{ran}(\Lambda - \lambda I) = \mathscr{G}$. The *spectrum* $\mathrm{spec}\,\Lambda$ of Λ is defined as

$$\mathrm{spec}\,\Lambda := \mathbb{C} \setminus \mathrm{res}\,\Lambda.$$

A linear relation Λ on $\mathscr{G}$ is called *symmetric* if $\Lambda \subset \Lambda^*$ and is called *self-adjoint* if $\Lambda = \Lambda^*$. A linear operator L in $\mathscr{G}$ is symmetric (respectively, self-adjoint) if and only if its graph is a symmetric (respectively, self-adjoint) linear relation. A self-adjoint linear relation is always maximal symmetric, but the converse in not true; examples are given by the graphs of maximal symmetric operators with deficiency indices $(\mathfrak{n},0)$, $\mathfrak{n} > 0$.

To describe all self-adjoint linear relations we need the following auxiliary result.

Lemma 1.1. *Let U be a unitary operator in $\mathscr{G}$. Then the operator $M : \mathscr{G} \oplus \mathscr{G} \to \mathscr{G} \oplus \mathscr{G}$,*

$$M = \frac{1}{2}\begin{pmatrix} i(1+U) & U-1 \\ 1-U & i(1+U) \end{pmatrix} \tag{1.1}$$

is unitary; in particular, $0 \in \mathrm{res}\,M$.

Proof. The adjoint operator M^* has the form

$$M^* = \frac{1}{2}\begin{pmatrix} -i(1+U^*) & 1-U^* \\ U^*-1 & -i(1+U^*) \end{pmatrix},$$

and it is easy to show by direct calculation that $M^* = M^{-1}$. □

Theorem 1.2. *A linear relation Λ in $\mathscr{G}$ is self-adjoint iff there is a unitary operator U in $\mathscr{G}$ (called the* Cayley transform *of Λ) such that*

$$\Lambda = \big\{ (x_1,x_2) \in \mathscr{G} \oplus \mathscr{G} : i(1+U)x_1 = (1-U)x_2 \big\}. \tag{1.2}$$

Writing U in the form $U = \exp(-2iA)$ with a self-adjoint operator A one can reformulate theorem 1.2 as follows:

Corollary 1.3. *A linear relation Λ in $\mathscr{G}$ is self-adjoint iff there is a self-adjoint operator A acting in $\mathscr{G}$ such that $\Lambda = \big\{ (x_1,x_2) \in \mathscr{G} \oplus \mathscr{G} : \cos A x_1 = \sin A x_2 \big\}$.*

To prove theorem 1.2 we need the following lemma.

Lemma 1.4. *Let U be a unitary operator in $\mathscr{G}$ and Λ be defined by (1.2), then*

$$\Lambda = \big\{ ((1-U)x, i(1+U)x) : x \in \mathscr{G} \big\}. \tag{1.3}$$

Proof of lemma 1.4. The linear relation Λ given by (1.2) is closed as it is the null space of the bounded operator

$$\mathscr{G} \oplus \mathscr{G} \ni (x_1,x_2) \mapsto i(1+U)x_1 - (1-U)x_2 \in \mathscr{G}.$$

Denote the set on the right-hand side of (1.3) by Π. Clearly, $\Pi \subset \Lambda$. By lemma 1.1, the operator M^* adjoint to M from (1.1) maps closed sets to closed sets. In particular, the subspace $\Pi \equiv M^*(0 \oplus \mathscr{G})$ is closed. Assume that there exists $(y_1,y_2) \in \Lambda$ such that $(y_1,y_2) \perp \Pi$. The condition $(y_1,y_2) \in \Lambda$ reads as $i(1+U)y_1 - (1-U)y_2 = 0$, and $(y_1,y_2) \perp \Pi$ means that $\langle y_1 | (1-U)x \rangle + \langle y_2 | i(1+U)x \rangle = 0$ for all $x \in \mathscr{G}$, i.e. that $(U-1)y_1 - i(1+U)y_2 = 0$. This implies $M(y_1,y_2) = 0$. By lemma 1.1, $y_1 = y_2 = 0$. The requested equality $\Lambda = \Pi$ is proved. □

Proof of theorem 1.2. (1) Let U be a unitary operator in $\mathscr{G}$ and Λ be defined by (1.2). By lemma 1.4 one can represent Λ in the form (1.3). Using this representation one easily concludes that $\Lambda \subset \Lambda^*$, i.e. that Λ is symmetric.

Let $(y_1,y_2) \in \Lambda^*$. The equality $\langle x_1 | y_2 \rangle = \langle x_1 | y_2 \rangle$ for all $(x_1,x_2) \in \Lambda$ is equivalent to $\langle (1-U)x | y_2 \rangle = \langle i(1+U)x | y_1 \rangle$ for all $x \in \mathscr{G}$, from which $-i(1+U^{-1})y_1 = (1-U^{-1})y_2$ and $i(1+U)y_1 = (1-U)y_2$, i.e. $(y_1,y_2) \in \Lambda$. Therefore, $\Lambda^* \subset \Lambda$, which finally results in $\Lambda = \Lambda^*$.

(2) Let Λ be a self-adjoint linear relation in $\mathscr{G}$. Set $L_\pm := \{x_1 \pm ix_2 : (x_1, x_2) \in \Lambda\}$. Assume that for some (x_1, x_2) and (y_1, y_2) from Λ one has $x_1 + ix_2 = y_1 + iy_2$, then $(x_1 - y_1, x_2 - y_2) \in \Lambda$ and $x_1 - y_1 = -i(x_2 - y_2)$. At the same time, $0 = \mathrm{Im}\langle x_1 - y_1 | x_2 - y_2 \rangle = \mathrm{Im}\langle -i(x_2 - y_2) | (x_2 - y_2) \rangle = \mathrm{Im}\, i \|x_2 - y_2\|^2$, therefore, $x_2 = y_2$ and $x_1 = y_1$. In the same way one can show that from $x_1 - ix_2 = y_1 - iy_2$, $(x_1, x_2), (y_1, y_2) \in \Lambda$, it follows that $x_1 = y_1$ and $x_2 = y_2$. For $x_1 + ix_2$ with $(x_1, x_2) \in \Lambda$ set $U(x_1 + ix_2) = x_1 - ix_2$. Clearly, $U : L_+ \to L_-$ is well-defined and bijective. Moreover, $\|U(x_1 + ix_2)\|^2 = \|x_1\|^2 + \|x_2\|^2 = \|x_1 + ix_2\|^2$, i.e. U is isometric.

Show that U is actually a unitary operator, i.e. that $L_\pm = \mathscr{G}$. We consider only L_+; the set L_- can be considered exactly in the same way. Assume that $y \perp L_+$ for some $y \in \mathscr{G}$, then $\langle x_1 + ix_2 | y \rangle = \langle x_1 | y \rangle - \langle x_2 | iy \rangle = 0$ for all $(x_1, x_2) \in \Lambda$. It follows that $(iy, y) \in \Lambda^* = \Lambda$, which implies $\mathrm{Im}\langle iy | y \rangle = -\mathrm{Im}\, i \|y\|^2 = 0$, i.e. $y = 0$. Therefore, $\overline{L_+} = \mathscr{G}$. To show that L_+ is closed we take an arbitrary sequence $(x_1^n, x_2^n) \in \Lambda$ with $\lim(x_1^n + ix_2^n) = y$ for some $y \in \mathscr{G}$, then automatically $\lim(x_1^n - ix_2^n) = y'$ for some $y' \in \mathscr{G}$, and

$$\lim x_1^n = \frac{1}{2}(y + y') =: y_1 \text{ and } \lim x_2^n = \frac{1}{2i}(y - y') =: y_2.$$

As we see, the sequence (x_1^n, x_2^n) converges, and the limit (y_1, y_2) lies in Λ as Λ is closed. Therefore, $y = y_1 + iy_2$ lies in L_+, L_+ is closed, and U is unitary.

Clearly, by construction of U, Λ is a subset of the subspace on the right-hand side of (1.2). As shown in item (1), the latter is self-adjoint as well as Λ is, therefore, they coincide. $\qquad\square$

Theorem 1.2 gives only one possible way for parameterizing linear relations with the help of operators. Let us mention some other ways to to this.

Proposition 1.5. *Let A and B be bounded linear operators in $\mathscr{G}$. Denote $\Lambda := \big\{(x_1, x_2) \in \mathscr{G} \oplus \mathscr{G} : Ax_1 = Bx_2\big\}$. Λ is self-adjoint iff the following two conditions are satisfied:*

$$AB^* = BA^*, \tag{1.4a}$$

$$\ker \begin{pmatrix} A & -B \\ B & A \end{pmatrix} = 0. \tag{1.4b}$$

Proof. Introduce operators $L : \mathscr{G} \oplus \mathscr{G} \ni (x_1, x_2) \mapsto Ax_1 - Bx_2 \in \mathscr{G}$ and $J : \mathscr{G} \oplus \mathscr{G} \ni (x_1, x_2) \mapsto (-x_2, x_1) \in \mathscr{G} \oplus \mathscr{G}$. There holds $\Lambda^* = J(\Lambda^\perp)$ and $\Lambda = \ker L$.

Let us show first that the condition (1.4a) is equivalent to the inclusion $\Lambda^* \subset \Lambda$. Note that this inclusion is equivalent to $J(\Lambda^\perp) \subset \Lambda$ or, due to the bijectivity of J, to

$$\Lambda^\perp \subset J\Lambda. \tag{1.5}$$

Clearly, $\Lambda \equiv \ker L$ is closed, therefore, by the well known relation, $\Lambda^\perp = \ker L^\perp = \overline{\operatorname{ran} L^*}$. As Λ is closed, the condition (1.5) is equivalent to

$$\operatorname{ran} L^* \subset J(\ker L). \tag{1.6}$$

Noting that L^* acts as $\mathscr{G} \ni x \mapsto (A^* x, -B^* x) \in \mathscr{G} \oplus \mathscr{G}$, we see that (1.6) is equivalent to (1.4a).

Now let Λ be self-adjoint, then $J(\Lambda^\perp) = \Lambda$ or, equivalently, $J(\Lambda) = \Lambda^\perp \equiv \ker L^\perp$. Therefore, the restriction of L to $J(\Lambda)$ is injective. This means that the systems of equations $Lz = 0$, $LJz = 0$ has only the trivial solution, which is exactly the condition (1.4b).

On the other hand, if (1.4a) and (1.4b) are satisfied, then, as shown above, $\Lambda^\perp \subset J(\Lambda)$. If $\Lambda^\perp \neq J(\Lambda)$, then $J(\Lambda)$ contains a non-zero element of $(\Lambda^\perp)^\perp \equiv \Lambda = \ker L$, i.e. there exists $z \neq 0$ with $Lz = 0$ and $LJz = 0$, which contradicts (1.4b). $\quad\square$

For a finite-dimensional $\mathscr{G}$ the condition (1.4b) simplifies, and one arrives at

Corollary 1.6. *Let $\mathscr{G}$ be finite dimensional, A, B be linear operators in $\mathscr{G}$. The linear relation $\Lambda := \big\{ (x_1, x_2) \in \mathscr{G} \oplus \mathscr{G} : Ax_1 = Bx_2 \big\}$ is self-adjoint iff the following two conditions are satisfied:*

$$AB^* = BA^*, \tag{1.7a}$$

$$\det(AA^* + BB^*) \neq 0 \quad \Leftrightarrow \quad \textit{the block matrix } (A|B) \textit{ has maximal rank.} \tag{1.7b}$$

The conditions (1.4a), (1.4b), (1.7a), (1.7b) can be rewritten in many equivalent forms, see e.g. [4, Section 125], [31, 47, 107, 118].

1.2 Boundary triples for linear operators

Definition 1.7. Let A be a closed linear operator in a Hilbert space $\mathscr{H}$ with the domain $\operatorname{dom} A$. Assume that there exist another Hilbert space $\mathscr{G}$ and two linear maps $\Gamma_1, \Gamma_2 : \operatorname{dom} A \to \mathscr{G}$ such that:

$$\langle f | Ag \rangle - \langle Af | g \rangle = \langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle \text{ for all } f, g \in \operatorname{dom} A, \tag{1.8a}$$

$$\text{the map } (\Gamma_1, \Gamma_2) : \operatorname{dom} A \to \mathscr{G} \oplus \mathscr{G} \text{ is surjective,} \tag{1.8b}$$

$$\text{the set } \ker (\Gamma_1, \Gamma_2) \text{ is dense in } \mathscr{H}. \tag{1.8c}$$

A triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$ with the above properties is called a *boundary triple* for A.

Remark 1.8. This definition differs slightly from the commonly used one. In [49, 71, 88] one defines boundary triple only for the case when A^* is a closed densely defined symmetric operator; the property (1.8c) holds then automatically. In our opinion, in some cases it is more convenient to find a boundary triple than to check whether the adjoint operator is symmetric. Below we will see (theorem 1.12) that these definitions are actually equivalent if one deals with self-adjoint extensions.

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In Definition 1.7, we do not assume any continuity properties of the maps Γ_1 and Γ_2, but they appear automatically.

Proposition 1.9. *Let A be a closed linear operator in a Hilbert space $\mathscr{H}$ and $(\mathscr{G}, \Gamma_1, \Gamma_2)$ be its boundary triple, then the mapping $\operatorname{dom} S \ni g \mapsto (\Gamma_1 g, \Gamma_2 g) \in \mathscr{G} \oplus \mathscr{G}$ is continuous with respect to the graph norm of S.*

Proof. Suppose that a sequence $g_n \in \operatorname{dom} A$, $n \in \mathbb{N}$, converges in the graph norm. As A is closed, there holds $g := \lim g_n \in \operatorname{dom} A$ and $Ag = \lim Ag_n$. Assume that $\lim(\Gamma_1 g_n, \Gamma_2 g_n) = (u, v)$, where the limit is taken in the norm of $\mathscr{G} \oplus \mathscr{G}$. Let us show that $\Gamma_1 g = u$ and $\Gamma_2 g = v$; this will mean that the mapping (Γ_1, Γ_2) is closed and, therefore, continuous by the closed graph theorem.

For an arbitrary $f \in \operatorname{dom} A$ there holds

$$\begin{aligned}
\langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle &= \langle f | Ag \rangle - \langle Af | g \rangle \\
&= \lim \langle f | Ag_n \rangle - \langle Af | g_n \rangle = \lim \langle \Gamma_1 f | \Gamma_2 g_n \rangle - \langle \Gamma_2 f | \Gamma_1 g_n \rangle \\
&= \langle \Gamma_1 f | v \rangle - \langle \Gamma_2 f | u \rangle.
\end{aligned}$$

Therefore, $\langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle = \langle \Gamma_1 f | v \rangle - \langle \Gamma_2 f | u \rangle$ and

$$\langle \Gamma_1 f | \Gamma_2 g - v \rangle = \langle \Gamma_2 f | \Gamma_1 g - u \rangle \tag{1.9}$$

for any $f \in \operatorname{dom} A$. Using the property (1.8b) from definition 1.7, one can take $f \in \operatorname{dom} A$ with $\Gamma_1 f = \Gamma_2 g - v$ and $\Gamma_2 f = 0$, then (1.9) reads as $\|\Gamma_2 g - v\|^2 = 0$ and $\Gamma_2 g = v$. Analogously, choosing $f \in \operatorname{dom} A$ with $\Gamma_1 f = 0$ and $\Gamma_2 f = \Gamma_1 g - u$ one arrives at $\Gamma_1 g = u$. $\qquad\square$

Our next aim is to describe situations in which boundary triples exist and are useful. For a symmetric operator A in a Hilbert space $\mathscr{H}$ and for $z \in \mathbb{C}$, we denote throughout the paper $\mathscr{N}_z(A) := \ker(A^* - zI)$ and write sometimes $\mathscr{N}_z$ instead of $\mathscr{N}_z(A)$, if it does not lead to confusion.

Is is well known that A has self-adjoint extensions if and only if $\dim \mathscr{N}_i = \dim \mathscr{N}_{-i}$. The von Neumann theory states a bijection between the self-adjoint extensions and unitary operators from $\mathscr{N}_i$ to $\mathscr{N}_{-i}$. More precisely, if U is a unitary operator from $\mathscr{N}_i$ to $\mathscr{N}_{-i}$, then the corresponding self-adjoint extension A_U has the domain $\{f = f_0 + f_i + U f_i : f_0 \in \operatorname{dom} A, f_i \in \mathscr{N}_i\}$ and acts as $f_0 + f_i + U f_i \mapsto A f_0 + i f_i - i U f_i$. This construction is difficult to use in practical applications, and our aim is to show that the boundary triples provide a useful machinery for working with self-adjoint extensions.

The following proposition is borrowed from [88].

Proposition 1.10. *Let A be a densely defined closed symmetric operator in a Hilbert space $\mathscr{H}$ with equal deficiency indices $(\mathfrak{n}, \mathfrak{n})$, then there is a boundary triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$ for the adjoint A^* with $\dim \mathscr{G} = \mathfrak{n}$.*

Proof. It is well known that $\operatorname{dom} A^* = \operatorname{dom} A + \mathscr{N}_i + \mathscr{N}_{-i}$, and this sum is direct. Let $P_{\pm i}$ be the projector from $\operatorname{dom} A^*$ to $\mathscr{N}_{\pm i}$ corresponding to this expansion.

Let $f, g \in \operatorname{dom} A^*$, then $f = f_0 + P_i f + P_{-i} f$, $g = g_0 + P_i g + P_{-i} g$, $f_0, g_0 \in \operatorname{dom} A$. Using the equalities $A^* P_i = i P_i$ and $A^* P_{-i} = -i P_{-i}$ one obtains

$$
\langle f | A^* g \rangle - \langle A^* f | g \rangle = \langle f_0 + P_i f + P_{-i} f | A g_0 + i P_i g - i P_{-i} g \rangle
$$
$$
= 2i \langle P_i f | P_i g \rangle - 2i \langle P_{-i} f | P_{-i} g \rangle. \quad (1.10)
$$

As the deficiency indices of A are equal, there is an isomorphism U from $\mathscr{N}_{-i}$ onto $\mathscr{N}_i$. Denote $\mathscr{G} := \mathscr{N}_{-i}$ endowed with the induced scalar product in $\mathscr{H}$, and set $\Gamma_1 = iUP_{-i} - iP_i$, $\Gamma_2 = P_i + UP_{-i}$, then

$$
\langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle = 2i \langle P_i f | P_i g \rangle - 2i \langle UP_{-i} f | UP_{-i} g \rangle
$$
$$
= 2i \langle P_i f | P_i g \rangle - 2i \langle P_{-i} f | P_{-i} g \rangle. \quad (1.11)
$$

Comparing (1.10) with (1.11) one shows that $(\mathscr{G}, \Gamma_1, \Gamma_2)$ satisfy the property (1.8a) of definition (1.7). Due to $\operatorname{dom} A \subset \ker(P_i, P_{-i}) \subset \ker(\Gamma_1, \Gamma_2)$ the property (1.8c) is satisfied too. To prove (1.8b) take any $F_1, F_2 \in \mathscr{N}_{-i} \equiv \mathscr{G}$ and show that the system of equations

$$
iUP_{-i} f - iP_i f = F_1, \quad UP_{-i} f + P_i f = F_2, \quad (1.12)
$$

has a solution $f \in \operatorname{dom} A^*$. Multiplying the second equation by i and adding it to the first one one arrives at $2iUP_{-i} f = F_1 + iF_2$. In a similar way, $2iP_i f = iF_2 - F_1$. Therefore, the funtcion

$$
f = \frac{1}{2i}(iF_2 - F_1) + \frac{1}{2i}U^{-1}(F_1 + iF_2) \in \mathscr{N}_i(A^*) + \mathscr{N}_{-i}(A^*) \subset \operatorname{dom} A^*
$$

is a possible solution to (1.12), and (1.8b) is satisfied. Therefore, $(\mathscr{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for A^*. $\qquad\qquad \square$

Let A be a closed densely defined linear operator, A^* have a boundary triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$, Λ be a closed linear relation in $\mathscr{G}$. By A_Λ in *this subsection* we mean the restriction of A^* to the domain $\operatorname{dom} A_\Lambda = \{f \in \operatorname{dom} A^* : (\Gamma_1 f, \Gamma_2 f) \in \Lambda\}$.

The usefulness of boundary triples is described in the following proposition.

Proposition 1.11. *For any closed linear relation Λ in $\mathscr{G}$ one has $A_\Lambda^* = A_{\Lambda^*}$. In particular, A_Λ is symmetric/self-adjoint if and only if Λ is symmetric/self-adjoint, respectively.*

Proof. Clearly, one has $A \subset A_\Lambda \subset A^*$. Therefore, $A \subset A_\Lambda^* \subset A^*$. Moreover, one has

$$
\begin{aligned}
\operatorname{gr} A_\Lambda^* &= \{(f, A^* f) : \langle f | A^* g \rangle = \langle A^* f | g \rangle \quad \forall g \in \operatorname{dom} A_\Lambda \} \\
&= \{(f, A^* f) : \langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle \quad \forall g \in \operatorname{dom} A_\Lambda \} \\
&= \{(f, A^* f) : \langle \Gamma_1 f | x_2 \rangle - \langle \Gamma_2 f | x_1 \rangle \quad \forall (x_1, x_2) \in \Lambda \} \\
&= \{(f, A^* f) : (\Gamma_1 f, \Gamma_2 f) \in \Lambda^* \} = \operatorname{gr} A_{\Lambda^*}.
\end{aligned}
$$

This proves the first part of proposition. The part concerning the self-adjointness of A_Λ is now obvious, as $A_\Lambda \subset A_{\Lambda'}$ if and only if $\Lambda \subset \Lambda'$. $\qquad \square$

Theorem 1.12. *Let A be a closed densely defined symmetric operator.*

(1) The operator A^* has a boundary triple if and only if A admits self-adjoint extensions.

(2) If $(\mathcal{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for A^*, then there is a one-to-one correspondence between all self-adjoint linear relations Λ in $\mathcal{G}$ and all self-adjoint extensions of A given by $\Lambda \leftrightarrow A_\Lambda$, where A_Λ is the restriction of A^* to the vectors $f \in \operatorname{dom} A^*$ satisfying $(\Gamma_1 f, \Gamma_2 f) \in \Lambda$.

Proof. (1) Let A^* have a boundary triple and Λ be any self-adjoint linear relation in $\mathcal{G}$, then according to proposition 1.11 the operator A_Λ is self-adjoint, and $A_\Lambda \supset A$. The converse is exactly proposition 1.10.

(2) If Λ is a self-adjoint linear relation in $\mathcal{G}$, then due to proposition 1.11 the corresponding operator A_Λ is self-adjoint.

Now let B be a self-adjoint extension of A, then $A \subset B \subset A^*$. Denote $\Lambda = \{(\Gamma_1 f, \Gamma_2 f), f \in \operatorname{dom} B^*\}$, then $B = A_\Lambda$, and Λ is self-adjoint due to proposition 1.11. $\qquad \square$

Theorem 1.13. *Let a closed linear operator B have a boundary triple $(\mathcal{G}, \Gamma_1, \Gamma_2)$, and $A := B|_{\ker(\Gamma_1, \Gamma_2)}$, then $A \subset B^*$. Moreover, the following three conditions are equivalent:*

(1) B has at least one restriction which is self-adjoint,

(2) B^* is symmetric;

(3) $B^* = A$,

(4) $A^* = B$.

Proof. By construction A is densely defined. By definition 1.7 for any $f \in \mathrm{dom}\,A$ one has $\langle f | Bg \rangle - \langle Af | g \rangle = 0$, which means $A \subset B^*$. In particular, B^* is densely defined. By proposition 1.9, A is closed, therefore, (3) and (4) are equivalent.

(1)$\Rightarrow$(2). Let C be a self-adjoint restriction of B. From $C \subset B$ it follows $B^* \subset C^* \equiv C \subset B \equiv (B^*)^*$, i.e. B^* is symmetric.

(2)$\Rightarrow$(3). Let $D = B^*$ be symmetric, then $D \subset B$ is closed and $B = D^*$.

Let $f \in \mathrm{dom}\,D$. According to the definition 1.7 there exists $g \in \mathrm{dom}\,D^* = \mathrm{dom}\,B$ with $\Gamma_1 g = -\Gamma_2 f$ and $\Gamma_2 g = \Gamma_1 f$. One has

$$0 = \langle Df | g \rangle - \langle Df | g \rangle = \langle f | D^* g \rangle - \langle D^* f | g \rangle$$
$$\equiv \langle f | Bg \rangle - \langle Bf | g \rangle = \|\Gamma_1 f\|^2 + \|\Gamma_2 f\|^2,$$

from which $\Gamma_1 f = \Gamma_2 f = 0$. Therefore, $\mathrm{dom}\,D \subset \ker(\Gamma_1, \Gamma_2) \equiv \mathrm{dom}\,A$. At the same time, as shown above, $A \subset B^*$, which means $A = D = B^*$.

(4)$\Rightarrow$(1). Let $B = A^*$. By theorem 1.12(1) the operator A has self-adjoint extensions, which are at the same time self-adjoint restrictions of $A^* = B$. $\square$

The proof of proposition 1.10 gives a possible construction of a boundary triple. Clearly, boundary triple is not fixed uniquely by definition 1.7. For a description of all possible boundary triple we refer to [100, 101]. We restrict ourselves by the following observations.

Proposition 1.14. *Let A be a closed densely defined symmetric operator with equal deficiency indices. For any self-adjoint extension H of A there exists a boundary triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$ for A^* such that H is the restriction of A^* to $\ker \Gamma_1$.*

Proof. Let $(\mathscr{G}, \Gamma_1', \Gamma_2')$ be an arbitrary boundary triple for A^*. According to theorem 1.12(2), there exists a self-adjoint linear relation Λ in $\mathscr{G}$ such that H is the restriction of A^* to the vectors $f \in \mathrm{dom}\,A^*$ satisfying $(\Gamma_1' f, \Gamma_2' f) \in \Lambda$. Let U be the Cayley transform of Λ (see theorem 1.2). Set

$$\Gamma_1 := \frac{1}{2}\left(i(1+U)\Gamma_1' + (U-1)\Gamma_2'\right), \quad \Gamma_2 := \frac{1}{2}\left((1-U)\Gamma_1' + i(1+U)\Gamma_2'\right).$$

By lemma 1.1 the map $(\Gamma_1, \Gamma_2) : \mathrm{dom}\,A^* \to \mathscr{G} \oplus \mathscr{G}$ is surjective and $\ker(\Gamma_1, \Gamma_2) = \ker(\Gamma_1', \Gamma_2')$. At the same time one has $\langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle \equiv \langle \Gamma_1' f | \Gamma_2' g \rangle - \langle \Gamma_2' f | \Gamma_1' g \rangle$, which means that $(\mathscr{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for A^*. It remains to note that the conditions $(\Gamma_1' f, \Gamma_2' f) \in \Lambda$ and $\Gamma_1 f = 0$ are equivalent by the choice of U. $\square$

Proposition 1.15. *Let $(\mathscr{G}, \Gamma_1, \Gamma_2)$ be an arbitrary boundary triple for A^*, and L be a bounded linear self-adjoint operator in $\mathscr{G}$, then $(\mathscr{G}, \widetilde{\Gamma}_1, \widetilde{\Gamma}_2)$ with $\widetilde{\Gamma}_1 = \Gamma_1$ and $\widetilde{\Gamma}_2 = \Gamma_2 + L\Gamma_1$ is also a boundary triple for S^*.*

Proof. The conditions of definition 1.7 are verified directly. $\qquad\square$

An explicit construction of boundary triples is a rather difficult problem, see e.g. [124] for the discussion of elliptic boundary conditions. In some cases there are natural boundary triples reflecting some specific properties of the problem, like in the theory of singular perturbations, see [114] and subsection 1.4.2 below.

1.3 Krein's resolvent formula

In this subsection, if not specified explicitly,

- S is a densely defined symmetric operator with equal deficiency indices $(\mathfrak{n},\mathfrak{n})$, $0 < \mathfrak{n} \le \infty$, in a Hilbert space $\mathscr{H}$,

- $\mathscr{N}_z := \ker(S^* - z)$,

- $\mathscr{G}$ is a Hilbert space of dimension $\mathfrak{n}$,

- H^0 is a certain self-adjoint extension of S,

- for $z \in \operatorname{res} H^0$ denote $R^0(z) := (H^0 - z)^{-1}$, the resolvent of H^0.

For $z_1, z_2 \in \operatorname{res} H^0$ put

$$U(z_1, z_2) = (H^0 - z_2)(H^0 - z_1)^{-1} \equiv 1 + (z_1 - z_2)R^0(z_1).$$

It is easy to show that $U(z_1, z_2)$ is a linear topological isomorphism of $\mathscr{H}$ obeying the following properties:

$$U(z,z) = I, \tag{1.13a}$$
$$U(z_1, z_2)U(z_2, z_3) = U(z_1, z_3), \tag{1.13b}$$
$$U^{-1}(z_1, z_2) = U(z_2, z_1), \tag{1.13c}$$
$$U^*(z_1, z_2) = U(\bar{z}_1, \bar{z}_2), \tag{1.13d}$$
$$U(z_1, z_2)\mathscr{N}_{z_2}(S) = \mathscr{N}_{z_1}(S). \tag{1.13e}$$

Definition 1.16. A map $\gamma : \operatorname{res} H^0 \to \mathbf{L}(\mathscr{G}, \mathscr{H})$ is called a *Krein Γ-field* for $(S, H^0, \mathscr{G})$ if the following two conditions are satisfied:

$\gamma(z)$ is a linear topological isomorphism of $\mathscr{G}$ and $\mathscr{N}_z$ for all $z \in \operatorname{res} H^0$, (1.14a)

for any $z_1, z_2 \in \operatorname{res} H^0$ there holds $\gamma(z_1) = U(z_1, z_2)\gamma(z_2)$ or, equivalently, $\gamma(z_1) - \gamma(z_2) = (z_1 - z_2)R^0(z_1)\gamma(z_2) = (z_1 - z_2)R^0(z_2)\gamma(z_1)$. (1.14b)

Let us discuss questions concerning the existence and uniqueness of Γ-fields.

Proposition 1.17. *For any triple* $(S, H^0, \mathscr{G})$ *there exists a Krein* Γ-*field* γ. *If* $\widetilde{\gamma}(z)$ *is another Krein* Γ-*field for* $(S, H^0, \widetilde{\mathscr{G}})$ *with a certain Hilbert space* $\widetilde{\mathscr{G}}$, *then there exists a linear topological isomorphism* N *from* $\widetilde{\mathscr{G}}$ *to* $\mathscr{G}$ *such that* $\widetilde{\gamma}(z) = \gamma(z)N$.

Proof. Fix any $z_0 \in \mathrm{res}\, H^0$, choose any linear topological isomorphism $L : \mathscr{G} \to \mathcal{N}_{z_0}$, and set $\gamma(z_0) := L$. Then property (1.14b) forces to set

$$\gamma(z) = U(z, z_0)L \equiv L + (z - z_0)R^0(z)L. \tag{1.15}$$

On the other hand, the properties (1.13) of $U(z_1, z_2)$ show that $\gamma(z)$ defined by (1.15) is a Γ-field for $(S, H^0, \mathscr{G})$.

If $\widetilde{\gamma}(z) : \widetilde{\mathscr{G}} \to \mathscr{H}$, $z \in \mathrm{res}\, H^0$, is another Γ-field for $(S, H^0, \mathscr{G})$, then setting $N = \widetilde{\gamma}(z_0)\gamma^{(-1)}(z_0)$ where $\gamma^{(-1)}(z_0)$ is the inverse to $\gamma(z_0) : \mathscr{G} \to \mathcal{N}_{z_0}$, and using (1.14b) again, we see that $\widetilde{\gamma}(z) = \gamma(z)N$ for all $z \in \mathrm{res}\, H^0$. $\qquad\square$

The following propositions gives a characterization of all Krein Γ-fields.

Proposition 1.18. *Let* H^0 *be a self-adjoint operator in a Hilbert space* $\mathscr{H}$, $\mathscr{G}$ *be another Hilbert space, and* γ *be a map from* $\mathrm{res}\, H^0$ *to* $\mathbf{L}(\mathscr{G}, \mathscr{H})$, *then the following assertions are equivalent:*

(1) there is a closed densely defined symmetric restriction S *of* H^0 *such that* γ *is the* Γ-*field for* $(S, H^0, \mathscr{G})$.

(2) γ *satisfies the condition* (1.14b) *above and the following additional condition:*

> *for some* $\zeta \in \mathrm{res}\, H^0$ *the map* $\gamma(\zeta)$ *is a linear topological isomorphism of* $\mathscr{G}$ *on a subspace* $\mathcal{N} \subset \mathscr{H}$ *such that* $\mathcal{N} \cap$ (1.16) $\mathrm{dom}\, H^0 = \{0\}$.

Proof. Clearly, any Γ-field satisfies (1.16).

Conversely, let the conditions (1.16) and (1.14b) be fulfilled for a map $\gamma : \mathrm{res}\, H^0 \to \mathbf{L}(\mathscr{G}, \mathscr{H})$. Then, in particular, $\gamma(z)$ is a linear topological isomorphism on a subspace of $\mathscr{H}$ for any $z \in \mathrm{res}\, H^0$. Denote $\mathscr{D}_z = \ker \gamma^*(z)(H^0 - \bar{z})$. According to (1.14b) we have for any $z_1, z_2 \in \mathrm{res}\, H^0$

$$\gamma^*(z_2) = \gamma^*(z_1)U^*(z_2, z_1) = \gamma^*(z_1)(H^0 - \bar{z}_1)(H^0 - \bar{z}_2)^{-1}.$$

Hence $\gamma^*(z_2)(H^0 - \bar{z}_2) = \gamma^*(z_1)(H^0 - \bar{z}_1)$, therefore $\mathscr{D}_z$ is independent of z. Denote $\mathscr{D} := \mathscr{D}_z$ and define S as the restriction of H^0 to $\mathscr{D}$. Show that $\mathscr{D}$ is dense in $\mathscr{H}$. Let $\varphi \perp \mathscr{D}$. Since $\mathscr{D} = \mathscr{D}_\zeta = R^0(\bar{\zeta})(\mathcal{N}^\perp)$, this means that $\langle R^0(\zeta)\varphi \,|\, \psi \rangle = 0$

for each $\psi \in \mathcal{N}^{\perp}$, i.e. we have $R^0(\zeta)\varphi \in \mathcal{N}$. Hence, $R^0(\zeta)\varphi = 0$, therefore $\varphi = 0$. Thus, S is densely defined. Let us show that

$$\operatorname{ran}(S - \bar{z}) = \ker \gamma^*(z) \tag{1.17}$$

for any $z \in \operatorname{res} H^0$. Let $\gamma^*(z)\varphi = 0$; set $\psi := (H^0 - \bar{z})^{-1}\varphi$, then $\psi \in \operatorname{dom} S \equiv \mathscr{D}$, therefore, $\varphi \in \operatorname{ran}(S - \bar{z})$. Conversely, if $\varphi \in \operatorname{ran}(S - \bar{z})$, then $\varphi = (S - \bar{z})\psi$ where $\gamma^*(z)(H^0 - \bar{z})\psi = 0$, and (1.17) is proven. In particular, (1.17) implies that S is closed. Moreover, we have from (1.17)

$$\mathcal{N}_z = \operatorname{ran}(S - \bar{z})^{\perp} = \ker \gamma^*(z)^{\perp} = \overline{\operatorname{ran} \gamma(z)} = \operatorname{ran} \gamma(z).$$

Thus, γ is a Γ-field for $(S, H^0, \mathscr{G})$. $\qquad \square$

Let now the triple $(S, H^0, \mathscr{G})$ be endowed with a Γ-field γ, $\gamma : \operatorname{res} H^0 \to \mathbf{L}(\mathscr{G}, \mathscr{H})$.

Definition 1.19. A map $Q : \operatorname{res} H^0 \to \mathbf{L}(\mathscr{G}, \mathscr{G})$ is called a *Krein $\mathscr{Q}$-function* for $(S, H^0, \mathscr{G}, \gamma)$, if

$$Q(z_1) - Q^*(\bar{z}_2) = (z_1 - z_2)\gamma^*(\bar{z}_2)\gamma(z_1) \text{ for any } z_1, z_2 \in \operatorname{res} H^0. \tag{1.18}$$

Proposition 1.20. *For any $(S, H^0, \mathscr{G})$ endowed with a Krein Γ-field γ there exists a Krein $\mathscr{Q}$-function $Q : \operatorname{res} H^0 \to \mathbf{L}(\mathscr{G}, \mathscr{G})$. If $\widetilde{Q}(z) : \mathscr{G} \to \mathscr{G}$, $z \in \operatorname{res} H^0$, is another $\mathscr{Q}$-function for $(S, H^0, \mathscr{G}, \gamma)$, then $\widetilde{Q}(z) = Q(z) + M$, where M is a bounded self-adjoint operator in $\mathscr{G}$.*

Proof. Fix as any $z_0 \in \operatorname{res} H^0$ and denote $x_0 := \operatorname{Re} z_0$, $y_0 := \operatorname{Im} z_0$, $L := \gamma(z_0)$. If a $\mathscr{Q}$-function exists, then by (1.18) one has $Q(z) = Q^*(z_0) + (z - \bar{z}_0)L^*\gamma(z)$. On the other hand

$$Q^*(z_0) = \frac{Q(z_0) + Q^*(z_0)}{2} - \frac{Q(z_0) - Q^*(z_0)}{2}.$$

Clearly, $Q(z_0) + Q^*(z_0)$ is a bounded self-adjoint operator in $\mathscr{G}$, denote it by $2C$. According to (1.18), $Q(z_0) - Q^*(z_0) = 2iy_0L^*L$, and therefore

$$Q(z) = C - iy_0L^*L + (z - \bar{z}_0)L^*\gamma(z). \tag{1.19}$$

We have from (1.19) that if $\widetilde{Q}(z)$ is another $\mathscr{Q}$-function for $(S, H^0, \mathscr{G}, \gamma)$, then $\widetilde{Q}(z) - Q(z) = M$ where M is a bounded self-adjoint operator which is independent of z.

It remains to show that a function of the form (1.19) obeys (1.18). Take arbitrary $z_1, z_2 \in \operatorname{res} H^0$. We have $Q^*(z_2) = C + iy_0L^*L + (\bar{z}_2 - z_0)\gamma^*(z_2)L$. Therefore,

$$Q(z_1) - Q^*(z_2) = (\bar{z}_0 - z_0)L^*L + (z - \bar{z}_0)L^*\gamma(z_1) + (z_0 - \bar{z}_2)\gamma^*(z_2)L. \tag{1.20}$$

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By (1.14b), $L = \gamma(z_0) = \gamma(z_1) + (z_0 - z_1)R^0(z_0)\gamma(z_1)$ and $L^* = \gamma^*(z_0) = \gamma^*(z_2) + (\bar{z}_0 - \bar{z}_2)\gamma^*(z_2)R^0(\bar{z}_0)$. Substituting these expressions in (1.20) we obtain

$$
\begin{aligned}
Q(z_1) - Q^*(z_2) = {} & (z_1 - \bar{z}_2)\gamma^*(z_2)\gamma(z_1) \\
& + \gamma^*(z_2)\Big\{ (\bar{z}_0 - z_0)\big[(\bar{z}_0 - \bar{z}_2)R^0(\bar{z}_0) + (z_0 - z_1)R^0(z_0) \\
& + (\bar{z}_0 - \bar{z}_2)(z_0 - z_1)R^0(\bar{z}_0)R^0(z_0)\big] + (z_1 - \bar{z}_0)(\bar{z}_0 - \bar{z}_2)R^0(\bar{z}_0) \\
& + (z_0 - \bar{z}_2)(z_0 - z_1)R^0(z_0)\Big\}\gamma(z_1).
\end{aligned}
$$

The expression in the curly brackets is equal to

$$
\begin{aligned}
& (\bar{z}_0 - z_0)(\bar{z}_0 - \bar{z}_2)R^0(\bar{z}_0) + (z_1 - \bar{z}_0)(\bar{z}_0 - \bar{z}_2)R^0(\bar{z}_0) \\
& + (z_0 - z_1)(\bar{z}_0 - \bar{z}_2)R^0(\bar{z}_0) + (\bar{z}_0 - z_0)(z_0 - z_1)R^0(z_0) \\
& + (z_0 - \bar{z}_2)(z_0 - z_1)R^0(z_0) - (\bar{z}_0 - \bar{z}_2)(z_0 - z_1)R^0(z_0).
\end{aligned}
$$

It is easy to see that the latter expression is equal to zero, and we get the result. $\square$

Below we list some properties of Γ-fields and $\mathscr{Q}$-functions which follow easily from the definitions.

Proposition 1.21. *Let γ be a Krein Γ-field for $(S, H^0, \mathscr{H})$, then γ is holomorphic in $\operatorname{res} H^0$ and satisfies*

$$
\frac{d}{dz}\gamma(z) = R^0(z)\gamma(z), \tag{1.21a}
$$

$$
S^*\gamma(z) = z\gamma(z), \tag{1.21b}
$$

$$
\gamma^*(z) \text{ is a bijection from } \mathscr{N}_z \text{ onto } \mathscr{G}, \tag{1.21c}
$$

$$
\gamma^*(z)f = 0 \text{ iff } f \perp \mathscr{N}_z, \tag{1.21d}
$$

$$
\gamma^*(\bar{z}_1)\gamma(z_2) = \gamma^*(\bar{z}_2)\gamma(z_1), \tag{1.21e}
$$

$$
\operatorname{ran}\big[\gamma(z_1) - \gamma(z_2)\big] \subset \operatorname{dom} H^0 \text{ for any } z_1, z_2 \in \operatorname{res} H^0. \tag{1.21f}
$$

Let in addition Q be a Krein $\mathscr{Q}$-function for $(S, H^0, \mathscr{G})$ and γ, then Q is holomorphic in $\operatorname{res} H^0$, and the following holds:

$$
\frac{d}{dz}Q(z) = \gamma^*(\bar{z})\gamma(z), \tag{1.22a}
$$

$$
Q^*(\bar{z}) = Q(z), \tag{1.22b}
$$

$$
\text{for any } z \in \mathbb{C} \setminus \mathbb{R} \text{ there is } c_z > 0 \text{ with } \frac{\operatorname{Im} Q(z)}{\operatorname{Im} z} \geq c_z. \tag{1.22c}
$$

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Remark 1.22. The property (1.22c) means that $\mathscr{Q}$–function is an operator-valued Nevanlinna function (or Herglotz function). This implies a number of possible relations to the measure theory, spectral theory etc., and such functions appear in many areas outside the extension theory, see e.g. [47, 49, 66, 68, 104, 105] and references therein.

Our next aim is to relate boundary triples in definition 1.7 to Krein's maps from definition 1.16.

Theorem 1.23. *Let S be a closed densely defined symmetric operator in a Hilbert space $\mathscr{H}$ with equal deficiency indices.*

(1) *For any self-adjoint extension H of S and any $z \in \operatorname{res} H$ there holds $\operatorname{dom} S^* = \operatorname{dom} H + \mathscr{N}_z$, and this sum is direct.*

(2) *Let $(\mathscr{G}, \Gamma_1, \Gamma_2)$ be a boundary triple for S^* and H^0 be the restriction of S^* to $\ker \Gamma_1$ which is self-adjoint due to theorem 1.12. Then:*

(2a) *for any $z \in \operatorname{res} H^0$ the restriction of Γ_1 to $\mathscr{N}_z$ has a bounded inverse $\gamma(z) : \mathscr{G} \to \mathscr{N}_z \subset \mathscr{H}$ defined everywhere,*

(2b) *this map $z \mapsto \gamma(z)$ is a Krein Γ-field for $(S, H^0, \mathscr{G})$,*

(2c) *the map $\operatorname{res} H^0 \ni z \mapsto Q(z) = \Gamma_2 \gamma(z) \in \mathbf{L}(\mathscr{G}, \mathscr{G})$ is a Krein $\mathscr{Q}$-function for $(S, H^0, \mathscr{G})$ and γ.*

(2d) *for any $f \in \operatorname{dom} H^0$ and $z \in \operatorname{res} H^0$ there holds $\gamma^*(\bar{z})(H^0 - z)f = \Gamma_2 f$.*

Proof. (1) Let $f \in \operatorname{dom} S^*$, Denote $f_0 := (H-z)^{-1}(S^* - z)f$. Clearly, $f_0 \in \operatorname{dom} H$. For $g := f - f_0$ one has $(S^* - z)g = (S^* - z)f - (S^* - z)(H-z)^{-1}(S^* - z)f \equiv (S^* - z)f - (H-z)(H-z)^{-1}(S^* - z)f = 0$, therefore, $g \in \ker(S^* - z) \equiv \mathscr{N}_z$.

Now assume that for some $z \in \operatorname{res} H$ one has $f_0 + g_0 = f_1 + g_1$ for some $f_0, f_1 \in \operatorname{dom} H$ and $g_0, g_1 \in \mathscr{N}_z$, then $f_0 - f_1 = g_1 - g_0 \in \mathscr{N}_z$ and $(H-z)(f_0 - f_1) = (S^* - z)(f_0 - f_1) = 0$. As $H - z$ is invertible, one has $f_0 = f_1$ and $g_0 = g_1$.

(2a) Due to condition (1.8b), $\Gamma_1(\operatorname{dom} S^*) = \mathscr{G}$. Due to $\Gamma_1(\operatorname{dom} H^0) = 0$ and item (1) one has $\Gamma_1(\mathscr{N}_z) = \mathscr{G}$. Assume that $\Gamma_1 f = 0$ for some $f \in \mathscr{N}_z$, then $f \in \operatorname{dom} H^0 \cap \mathscr{N}_z$ and $f = 0$ by item (1). Therefore, $\Gamma_1 : \mathscr{N}_z \to \mathscr{G}$ is a bijection and, moreover, Γ_1 is continuous in the graph norm of S^* by proposition 1.9. At the same time, the graph norm of S^* on $\mathscr{N}_z$ is equivalent to the usual norm in $\mathscr{H}$, which means that the restriction of Γ_1 to $\mathscr{N}_z$ is a bounded operator. The graph of this map is closed, and the inverse map is bounded by the closed graph theorem.

(2b) The property (1.14a) is already proved in item (2a). Take arbitrary $z_1, z_2 \in \operatorname{res} H^0$ and $\xi \in \mathscr{G}$. Denote $f = \gamma(z_1)\xi$ and $g = U(z_2, z_1)f \equiv f + (z_2 - z_1)R^0(z_2)f$. As $R^0(z_2)f \in \operatorname{dom} H^0$, there holds $\Gamma_1 R^0(z_2)f = 0$ and $\Gamma_1 g = \Gamma_1 f$. Clearly, $f \in \mathscr{N}_{z_1}$, and to prove property (1.14b) it is sufficient to show that $(S^* - z_2)g = 0$.

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But this follows from the chain $(S^* - z_2)g = (S^* - z_2)f + (z_2 - z_1)(S^* - z_2)(H^0 - z_2)^{-1}f = (S^* - z_2)f + (z_2 - z_1)(H^0 - z_2)(H^0 - z_2)^{-1}f = (S^* - z_1)f = 0$.

Therefore, γ satisfies both properties (1.14a) and (1.14b) in definition 1.16.

(2c) As $\gamma(z)$ is bounded by item (2a) and Γ_2 is bounded by proposition 1.9, the map $Q(z)$ is a bounded linear operator on $\mathbf{L}(\mathscr{G}, \mathscr{G})$. To prove property (1.18) take arbitrary $z_1, z_2 \in \mathrm{res}\, H$, $\phi, \psi \in \mathscr{G}$, and set $f := \gamma(\bar{z}_2)\phi$, $g := \gamma(z_1)\psi$. Clearly,

$$\langle f | S^* g \rangle - \langle f | S^* g \rangle - (z_1 - z_2)\langle f | g \rangle$$
$$= \langle f | (S^* - z_1)g \rangle - \langle (S^* - \bar{z}_2)f | g \rangle = 0. \quad (1.23)$$

At the same time one has

$$\langle f | g \rangle = \langle \gamma(\bar{z}_2)\phi | \gamma(z_1)\psi \rangle = \langle \phi | \gamma^*(\bar{z}_2)\gamma(z_1)\psi \rangle. \quad (1.24)$$

Moreover, using the equality $\Gamma_1 \gamma(z)\xi = \xi$, which holds for all $\xi \in \mathscr{G}$ and $z \in \mathrm{res}\, H^0$, one obtains

$$\langle f | S^* g \rangle - \langle f | S^* g \rangle = \langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle$$
$$= \langle \Gamma_1 \gamma(\bar{z}_2)\phi | \Gamma_2 \gamma(z_1)\psi \rangle - \langle \Gamma_2 \gamma(\bar{z}_2)\phi | \Gamma_1 \gamma(z_1)\psi \rangle$$
$$= \langle \phi | Q(z_1)\psi \rangle - \langle Q(\bar{z}_2)\phi | \psi \rangle = \langle \phi | [Q(z_1) - Q^*(\bar{z}_2)] \psi \rangle.$$

Therefore, Eqs. (1.23) and (1.24) read as

$$\langle \phi | [Q(z_1) - Q^*(\bar{z}_2)] \psi \rangle = \langle \phi | (z_1 - z_2)\gamma^*(\bar{z}_2)\gamma(z_1)\psi \rangle,$$

which holds for any $\phi, \psi \in \mathscr{G}$. This implies (1.18).

(2d) For any $\phi \in \mathscr{G}$ one has

$$\langle \phi | \gamma^*(\bar{z})(H^0 - z)f \rangle = \langle \gamma(\bar{z})\phi | (H^0 - z)f \rangle = \langle \gamma(\bar{z})\phi | S^* f \rangle - z\langle \gamma(\bar{z})\phi | f \rangle$$
$$= \langle S^* \gamma(\bar{z})\phi | f \rangle - z\langle \gamma(\bar{z})\phi | f \rangle + \langle \Gamma_1 \gamma(\bar{z})\phi | \Gamma_2 f \rangle - \langle \Gamma_2 \gamma(\bar{z})\phi | \Gamma_1 f \rangle$$
$$= \langle (S^* - \bar{z})\gamma(\bar{z})\phi | f \rangle + \langle \phi | \Gamma_2 f \rangle = \langle \phi | \Gamma_2 f \rangle,$$

i.e. $\Gamma_2 f = \gamma^*(\bar{z})(H^0 - z)f$. $\qquad \square$

Definition 1.24. The Krein Γ-field and $\mathscr{Q}$-function defined in theorem 1.23 will be called *induced* by the boundary triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$.

Remark 1.25. The $\mathscr{Q}$-function induced by a boundary triple is often called the *Weyl function* [5, 49].

Conversely, starting with given Krein maps one can construct a boundary triple.

Proposition 1.26. *Let γ be a Krein Γ-field for $(S, H^0, \mathscr{G})$. For any $z \in \mathrm{res}\, H^0$, represent $f \in \mathrm{dom}\, S^*$ as*

$$f = f_z + \gamma(z)F, \tag{1.25}$$

where $f_z \in \mathrm{dom}\, H^0$, $F \in \mathscr{G}$. For a fixed $z \in \mathrm{res}\, H^0$ define

$$\Gamma_1 f := F, \quad \Gamma_2 f := \frac{1}{2}\left(\gamma^*(\bar{z})(H^0 - z)f_z + \gamma^*(z)(H^0 - \bar{z})f_{\bar{z}}\right),$$

then $(\mathscr{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for S^*, and $\gamma(z)$ is the induced Γ-field.

For further references we formulate a simplified version of proposition 1.26 for the case when H^0 has gaps.

Corollary 1.27. *Let γ be a Krein Γ-field for $(S, H^0, \mathscr{G})$. Assume that H^0 has a gap, and $\lambda \in \mathrm{res}\, H^0 \cap \mathbb{R}$. Represent $f \in \mathrm{dom}\, S^*$ as $f = f_\lambda + \gamma(\lambda)F$, where $f_\lambda \in \mathrm{dom}\, H^0$, $F \in \mathscr{G}$. Define*

$$\Gamma_1 f := F, \quad \Gamma_2 f := \gamma^*(\lambda)(H^0 - \lambda)f_\lambda,$$

then $(\mathscr{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for S^*.

Proof of proposition 1.26. First of all note that the component F in (1.25) is independent of z. To see that it is sufficient to write f as $f_z + \left(\gamma(z) - \gamma(\lambda)\right)F + \gamma(\lambda)F$ and to use the uniqueness of this expansion and the inclusion $\left(\gamma(z) - \gamma(\lambda)\right)F \in \mathrm{dom}\, H^0$ following from (1.21f).

The property (1.8b) of boundary triples is obvious. From the equality $(H^0 - z)\,\mathrm{dom}\, S^\perp = \ker(S^* - \bar{z})$ and (1.21d) it follows that $\mathrm{dom}\, S \subset \ker(\Gamma_1, \Gamma_2)$, which proves (1.8c). To show (1.8a) we write

$$
\begin{aligned}
2\langle f | S^* g\rangle &- 2\langle S^* f | g\rangle \\
&= \langle f | (S^* - z)g\rangle + \langle f | (S^* - \bar{z})g\rangle - \langle (S^* - z)f | g\rangle - \langle (S^* - \bar{z})f | g\rangle \\
&= \langle f_{\bar{z}} + \gamma(\bar{z})\Gamma_1 f | (H^0 - z)g_z\rangle + \langle f_z + \gamma(z)\Gamma_1 f | (H^0 - \bar{z})g_{\bar{z}}\rangle \\
&\quad - \langle (H^0 - z)f_z | g_{\bar{z}} + \gamma(\bar{z})\Gamma_1 g\rangle - \langle (H^0 - \bar{z})f_z | g_z + \gamma(z)\Gamma_1 g\rangle \\
&= \langle f_{\bar{z}} | (H^0 - z)g_z\rangle + \langle f_z | (H^0 - \bar{z})g_{\bar{z}}\rangle - \langle (H^0 - \bar{z})f_{\bar{z}} | g_z\rangle - \langle (H^0 - z)f_z | g_{\bar{z}}\rangle \\
&\quad + \langle \Gamma_1 f | \gamma^*(\bar{z})(H^0 - z)g_z\rangle + \langle \Gamma_1 f | \gamma^*(z)(H^0 - \bar{z})g_{\bar{z}}\rangle \\
&\quad - \langle \gamma^*(\bar{z})(H^0 - z)f_z | \Gamma_1 g\rangle - \langle \gamma^*(z)(H^0 - \bar{z})f_z, \Gamma_1 g\rangle \\
&= 2\langle \Gamma_1 f | \Gamma_2 g\rangle - 2\langle \Gamma_2 f | \Gamma_1 g\rangle.
\end{aligned}
$$

To show that this boundary triple induces γ it is sufficient to note that $\Gamma_1 \gamma(z) = \mathrm{id}_\mathscr{G}$ and $\gamma(z)\Gamma_1 = \mathrm{id}_{\mathrm{dom}\, S^*}$. $\square$

Proposition 1.26 does not use any information on $\mathscr{Q}$-functions, and $\mathscr{Q}$-functions can be taken into account as follows.

Proposition 1.28. *Let γ be a Γ-field for $(S, H^0, \mathcal{G})$ and Q be an associated $\mathcal{Q}$-function, then there exists a boundary triple $(\mathcal{G}, \Gamma_1, \Gamma_2)$ for S^* which induces γ and Q.*

Proof. Let $(\mathcal{G}, \Gamma_1', \Gamma_2')$ be the boundary triple for S^* defined in proposition 1.26 and $\widetilde{Q}$ be the induced $\mathcal{Q}$-function. By proposition 1.20, there exists a bounded self-adjoint operator M on $\mathcal{G}$ with $Q(z) = \widetilde{Q}(z) + M$. Clearly, $(\mathcal{G}, \Gamma_1, \Gamma_2)$ with $\Gamma_1 = \Gamma_1'$ and $\Gamma_2 = \Gamma_2' + M\Gamma_1'$ is another boundary triple for S^* by proposition 1.15. On the other hand, γ is still the Γ-field induced by this new boundary triple, and the induced $\mathcal{Q}$-function, which is $\Gamma_2\gamma(z) \equiv \Gamma_2'\gamma(z) + M\Gamma_1'\gamma(z) \equiv \widetilde{Q}(z) + M$, coincides with $Q(z)$. $\qquad\square$

One of the most useful tools for the spectral analysis of self-adjoint extensions is the Krein resolvent formula described in the following theorem.

Theorem 1.29. *Let S be a closed densely defined symmetric operator with equal deficiency indices in a Hilbert space $\mathcal{H}$, $(\mathcal{G}, \Gamma_1, \Gamma_2)$ be a boundary triple for S^*, H^0 be the self-adjoint restriction of S^* to $\ker\Gamma_1$, γ and Q be the Krein Γ-field and $\mathcal{Q}$-function induced by the boundary triple. Let Λ be a self-adjoint linear relation in $\mathcal{G}$ and H_Λ be the restriction of S^* to the functions $f \in \mathrm{dom}\, S^*$ satisfying $(\Gamma_1 f, \Gamma_2 f) \in \Lambda$.*

(1) For any $z \in \mathrm{res}\, H^0$ there holds $\ker(H_\Lambda - z) = \gamma(z)\ker\left(Q(z) - \Lambda\right)$.

(2) For any $z \in \mathrm{res}\, H^0 \cap \mathrm{res}\, H_\Lambda$ there holds $0 \in \mathrm{res}\left(Q(z) - \Lambda\right)$ and

$$(H^0 - z)^{-1} - (H_\Lambda - z)^{-1} = \gamma(z)\left(Q(z) - \Lambda\right)^{-1}\gamma^*(\bar{z}).$$

(3) There holds $\mathrm{spec}\, H_\Lambda \setminus \mathrm{spec}\, H^0 = \left\{z \in \mathrm{res}\, H^0 : 0 \in \mathrm{spec}\left(Q(z) - \Lambda\right)\right\}$.

Proof. (1) Assume that $\phi \in \ker\left(\Lambda - Q(z)\right)$ then there exists $\psi \in \mathcal{G}$ such that $(\phi, \psi) \in \Lambda$ and $\psi - Q(z)\phi = 0$. This means the inclusion $(\phi, Q(z)\phi) \in \Lambda$. Consider the vector $F = \gamma(z)\phi$. Clearly, $(S^* - z)F = 0$. The condition $(\Gamma_1 F, \Gamma_2 F) \equiv (\phi, Q(z)\phi) \in \Lambda$ means that $F \in \mathrm{dom}\, H_\Lambda$ and $(H_\Lambda - z)F = 0$. Therefore, $\gamma(z)\ker\left(Q(z) - \Lambda\right) \subset \ker(H_\Lambda - z)$.

Conversely, let $F \in \ker(H_\Lambda - z)$, $z \in \mathrm{res}\, H^0$. Then also $(S^* - z)F = 0$ and by theorem 1.23(1) there exists $\phi \in \mathcal{G}$ with $F = \gamma(z)\phi$. Clearly, $(\phi, Q(z)\phi) \equiv (\Gamma_1 F, \Gamma_2 F) \in \Lambda$, i.e. there exist $\psi \in \mathcal{G}$ with $(\phi, \psi) \in \Lambda$ and $Q(z)\phi = \psi$. But this means $\phi \in \ker\left(Q(z) - \Lambda\right)$.

(2) Let $z \in \mathrm{res}\, H^0 \cap \mathrm{res}\, H_\Lambda$. Take any $h \in \mathcal{H}$ and denote $f := (H_\Lambda - z)^{-1}h$; clearly, $f \in \mathrm{dom}\, H_\Lambda$, and by theorem 1.23(1) there exist uniquely determined functions $f_z \in \mathrm{dom}\, H^0$ and $g_z \in \mathcal{N}_z$ with $f = f_z + g_z$. There holds $h = (H_\Lambda - z)f =$

$(S^* - z)f = (S^* - z)f_z + (S^* - z)g_z = (S^* - z)f_z = (H^0 - z)f_z$ and $f_z = (H^0 - z)^{-1}h$. Moreover, from $\Gamma_1 f_z = 0$ one has $\Gamma_1 f = \Gamma_1 g_z$, $g_z = \gamma(z)\Gamma_1 f$, and, therefore,

$$(H_\Lambda - z)^{-1}h = (H^0 - z)^{-1}h + \gamma(z)\Gamma_1 f. \qquad (1.26)$$

Applying to the both sides of the equality $f = f_z + \gamma(z)\Gamma_1 f$ the operator Γ_2 one arrives at $\Gamma_2 f = \Gamma_2 f_z + Q(z)\Gamma_1 f$ and

$$\Gamma_2 f - Q(z)\Gamma_1 f = \Gamma_2 f_z. \qquad (1.27)$$

When h runs through the whole space $\mathscr{H}$, then f_z runs through $\mathrm{dom}\, H^0$ and the values $\Gamma_2 f_z$ cover the whole space $\mathscr{G}$. At the same time, if f runs through $\mathrm{dom}\, H_\Lambda$, then the values $(\Gamma_1 f, \Gamma_2 f)$ cover the whole Λ. It follows then from (1.27) that $\mathrm{ran}\,(\Lambda - Q(z)) = \mathscr{G}$. On the other hand, by (1) one has $\ker(\Lambda - Q(z)) = 0$ and $0 \in \mathrm{res}\,(\Lambda - Q(z))$. From (1.27) one obtains

$$\Gamma_1 f = (\Lambda - Q(z))^{-1}\Gamma_2 f_z. \qquad (1.28)$$

By theorem 1.23(2d) there holds $\Gamma_2 f_z = \gamma^*(\bar{z})h$. Substituting this equality into (1.28) and then into (1.26) one arrives at the conclusion.

The item (3) follows trivially from the item (2). $\qquad \square$

Remark 1.30. Note that the operators H_Λ and H^0 satisfy $\mathrm{dom}\, H_\Lambda \cap \mathrm{dom}\, H^0 = \mathrm{dom}\, S$ iff Λ is a self-adjoint operator (i.e. is a single-valued); one says that H_Λ and H^0 are *disjoint* extensions of S. In this case the resolvent formula conains only operators and has the direct meaning. As we will see below, in this case one can obtain slightly more spectral information in comparison with the case when Λ is a linear relation, so it is useful to understand how to reduce the general case to the disjoint one.

Let T be the maximal common part of H^0 and H_Λ, i.e. the restriction of S^* to $\mathrm{dom}\, H^0 \cap \mathrm{dom}\, H_\Lambda$. Clearly, T is a closed symmetric operator,

$$\mathrm{dom}\, T = \{f \in \mathrm{dom}\, S^* : \Gamma_1 f = 0, \quad \Gamma_2 f \in \mathscr{L}\} \qquad (1.29)$$

where $\mathscr{L} = \ker(\Lambda^{-1})$ is a closed linear subspace of $\mathscr{G}$.

Lemma 1.31. *Let $\mathscr{L}$ be a closed linear subspace of $\mathscr{G}$ and T be defined by* (1.29), *then* $\mathrm{dom}\, T^* = \{f \in \mathrm{dom}\, S^* : \Gamma_1 f \in \mathscr{L}^\perp\}$.

Proof. It is clear that both T and T^* are restrictions of S^*. Hence, for any $f \in \mathrm{dom}\, T$ and $g \in \mathrm{dom}\, S^*$ one has

$$W(f, g) := \langle f | S^* g \rangle - \langle Tf | g \rangle = \langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle = \langle \Gamma_2 f | \Gamma_1 g \rangle.$$

As $\Gamma_2(\mathrm{dom}\, T) = \mathscr{L}$, one has $W(f, g) = 0$ for all f iff $\Gamma_1 g \perp \mathscr{L}$. $\qquad \square$

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Now one can construct a boundary triple for T^* starting from the boundary triple for S^*.

Theorem 1.32. *Let the assumptions of theorem 1.29 be satisfied. Let $\mathscr{L}$ be a closed subset of $\mathscr{G}$ and an operator T be defined by (1.29). Then $(\widetilde{\mathscr{G}}, \widetilde{\Gamma}_1, \widetilde{\Gamma}_2)$ is a boundary triple for T^*, where $\widetilde{\mathscr{G}} := \mathscr{L}^\perp$ with the induced scalar product, $\widetilde{\Gamma}_j := P\Gamma_j$, $j = 1, 2$, and P is the orthogonal projection onto $\widetilde{\mathscr{G}}$ in $\mathscr{G}$. The induced Γ-field $\widetilde{\gamma}$ and $\mathscr{Q}$-function $\widetilde{Q}$ are $\widetilde{\gamma}(z) := \gamma(z)P$, $\widetilde{Q}(z) := PQ(z)P$ considered as maps from $\widetilde{\mathscr{G}}$ to $\mathscr{N}_z$ and in $\widetilde{\mathscr{G}}$, respectively.*

Proof. Direct verification. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Returning to the operators H^0 and H_Λ one sees that, by construction, they are disjoint extensions of T, and in the notation of theorem 1.32 they are given by the boundary conditions $\widetilde{\Gamma}_1 f = 0$ and $\widetilde{\Gamma}_2 f = L\widetilde{\Gamma}_1 f$, respectively, where L is a certain self-adjoint operator in $\widetilde{\mathscr{G}}$. Using theorem 1.29 one can relate the resolvents of H^0 and H_Λ by

$$(H^0 - z)^{-1} - (H_\Lambda - z)^{-1} = \widetilde{\gamma}(z)\big(\widetilde{Q}(z) - L\big)^{-1}\widetilde{\gamma}^*(\bar{z})$$
$$= \gamma(z)P\big(PQ(z)P - L\big)^{-1}P\gamma^*(\bar{z}), \quad (1.30)$$

and $\operatorname{spec} H_\Lambda \setminus \operatorname{spec} H^0 = \big\{z \in \operatorname{res} H^0 : 0 \in \operatorname{spec}\big(PQ(z)P - L\big)\big\}$.

The operator L can be calculated, for example, starting from the Cayley transform of Λ (see proposition 1.2). Namely, let U_Λ be the Cayley transform of Λ, then, obviously, $\widetilde{\mathscr{G}} = \ker(1 - U_\Lambda)^\perp$. The Cayley transform of L is then of the form $U_L := PU_\Lambda P$ considered as a unitary operator in $\widetilde{\mathscr{G}}$, and $L = i(1 - U_L)^{-1}(1 + U_L)$.

Remark 1.33. For the case of a *simple* symmetric operator (that is, having no nontrivial invariant subspaces) one can describe the *whole* spectrum in terms of the limit values of the Weyl function, and not only the spectrum lying in gaps of a fixed self-adjoint extensions, see [17,24] for discussion. We note that, nevertheless, the simplicity of an operator is a quite rare property in multidimensional problems which is quite difficult to check.

Remark 1.34. It seems that the notion of boundary value triple appered first in the papers by Bruk [27] and Kochubei [88], although the idea goes back to the paper by Calkin [38]. The notion of a Γ-field and a $\mathscr{Q}$-function appeared first in [92,98], where they were used to describe the generalized resolvents of self-adjoint extensions. The relationship between the boundary triples and the resolvent formula in the form presented in theorems 1.23 and 1.29 was found by Derkach and Malamud, but it seems that the only existing discussion was in [50], which is hardly available, so we preferred to provide a complete proof here. The same scheme of the proof works in more abstract situations, see e.g. [46]. The forumula (1.30) is borrowed from [115], but we give a different proof.

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Remark 1.35. Theorem 1.29 shows that one can express the resolvents of *all* self-adjoint extensions of a certain symmetric operator through the resolvent of a *fixed* extension, more precisely, of the one corresponding to the boundary condition $\Gamma_1 f = 0$. On the other hand, proposition 1.14 shows that by a suitable choice of boundary triple one start with any extension. Formulas expressing $\mathcal{Q}$-functions associated with different extensions of the same operator can be found e.g. in [49, 67, 96].

In view of proposition 1.5 on the parameterization of linear relations it would be natural to ask whether one can rewrite the Krein resolvent formula completely in terms of operators without using linear relations. Namely, if a self-adjoint linear relation Λ is given in the form $\Lambda = \{(x_1, x_2) \in \mathcal{G} \oplus \mathcal{G}; \, Ax_1 = Bx_2\}$, where A and B are bounded linear operators satisfying (1.4a) and (1.4b), can one write an analogue of the Krein resolvent formula for H_Λ in terms of A and B? We formulate only here the main result referring to the recent work [107] for the proof.

Theorem 1.36. *Let the assumptions of theorem 1.29 be satisfied and A, B be bounded linear operators in $\mathcal{G}$ satisfying* (1.4a) *and* (1.4b). *Denote by $H^{A,B}$ the self-adjoint extension of S corresponding to the boundary conditions $A\Gamma_1 f = B\Gamma_2 f$, then*

(1) For any $z \in \operatorname{res} H^0$ there holds $\ker(H^{A,B} - z) = \gamma(z) \ker\big(BQ(z) - A\big)$.

(2) For any $z \in \operatorname{res} H^0 \cap \operatorname{res} H^{A,B}$ the operator $BQ(z) - A$ is injective and

$$(H^0 - z)^{-1} - (H^{A,B} - z)^{-1} = \gamma(z)\big(BQ(z) - A\big)^{-1} B\gamma^*(\bar{z}). \qquad (1.31)$$

(3) If A and B satisfy additionally the stronger condition

$$0 \in \operatorname{res} \begin{pmatrix} A & -B \\ B & A \end{pmatrix}, \qquad (1.32)$$

then $0 \in \operatorname{res}\big(BQ(z) - A\big)$ for all $z \in \operatorname{res} H^0 \cap \operatorname{res} H^{A,B}$, and, respectively, $\operatorname{spec} H^{A,B} \setminus \operatorname{spec} H^0 = \big\{ z \in \operatorname{res} H^0 : 0 \in \operatorname{spec}\big(BQ(z) - A\big)\big\}$.

Note that the condition (1.32) is satisfied if one uses the parameterization by the Cayley transform (theorem 1.2), i.e. $A = i(1 + U)$, $B = 1 - U$ with a unitary U, see proposition 1.1. Therefore, one can perform a "uniform" analysis of all self-adjoint extensions using the single unitary parameter U. Note that the above normalization condition is trivial for finite deficiency indices, hence the Krein formula has a particularly transparent form [10].

We note in conclusion that the resolvent formulas (1.30) and (1.31) provide two different ways of working with non-disjoint extensions, and thay can be obtained one from another [115].

1.4 Examples

Here we consider some situations in which boundary triples arise.

1.4.1 Sturm-Liouville problems

A classical example comes from the theory of ordinary differential operators. Let $V \in L^2_{\mathrm{loc}}(0,\infty)$ be real valued and, for simplicity, semibounded below. Denote by S_0 the closure of the operator $-\dfrac{d^2}{dx^2} + V$ with the domain $C_0^\infty(0,\infty)$ in the space $\mathscr{H} := L^2(0,\infty)$. It is well-known that the deficiency indices of S_0 are $(1,1)$. Using the integration by parts one can easily show that for the adjoint $S := S_0^*$ as a boundary triple one can take $(\mathbb{C}, \Gamma_1, \Gamma_2)$, $\Gamma_1 f = f(0)$, $\Gamma_2 f = f'(0)$. Denoting for $z \neq \mathbb{C}$ by ψ_z the unique L^2-solution to $-\psi_z'' + V\psi_z = z\psi_z$ with $\psi_z(0) = 1$ we arrive to the induced Krein Γ-field, $\gamma(z)\xi = \xi\psi_z$, and the induced $\mathcal{Q}$-function $Q(z) = \psi_z'(0)$, which is nothing but the Weyl-Titchmarsh function. Determining the spectral properties of the self-adjoint extensions of S_0 with the help of this function is a classical problem of the spectral analysis.

An analogous procedure can be done for Sturm-Louville operators on a segment. In $\mathscr{H} := L^2[a,b]$, $-\infty < a < b < \infty$ consider an operator S acting by the rule $f \mapsto -f'' + Vf$ with the domain $\mathrm{dom}\, S = H^2[a,b]$; here we assume that $V \in L^2[a,b]$ is real-valued. It is well-known that S is closed. By partial integration one easily sees that $(\mathscr{G}, \Gamma_1, \Gamma_2)$,

$$\mathscr{G} = \mathbb{C}^2, \quad \Gamma_1 f = \begin{pmatrix} f(a) \\ f(b) \end{pmatrix}, \quad \Gamma_2 f = \begin{pmatrix} f'(a) \\ -f'(b) \end{pmatrix},$$

is a boundary triple for S. The distinguisged extension H^0 corresponding to the boundary condition $\Gamma_1 f = 0$ is nothing but the operator $-d^2/dx^2 + V$ with the Dirichlet boundary conditions.

Let two functions $s(\cdot;z), c(\cdot;z) \in \ker(S - z)$ solve the equation

$$-f'' + Vf = zf, \quad z \in \mathbb{C}, \tag{1.33}$$

and satisfy $s(a;z) = c'(a;z) = 0$ and $s'(a;z) = c(a;z) = 1$. Clearly, s, c as well as their derivatives are entire functions of z; these solutions are linearly independent, and their Wronksian $w(z) \equiv s'(x;z)c(x;z) - s(x;z)c'(x;z)$ is equal to 1. For $z \notin \mathrm{spec}\, H^0$ one has $s(b;z) \neq 0$, and any solution f to (1.33) can be written as

$$f(x;z) = \frac{f(b) - f(a)c(b;z)}{s(b;z)} s(x;z) + f(a)c(x;z), \tag{1.34}$$

which means that the Γ-field induced by the above boundary triple is

$$\gamma(z) \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \frac{\xi_2 - \xi_1 c(b;z)}{s(b;z)} s(x;z) + \xi_1 c(x;z).$$

The calculation of $f'(a)$ and $-f'(b)$ gives

$$\begin{pmatrix} f'(a;z) \\ -f'(b;z) \end{pmatrix} = Q(z) \begin{pmatrix} f(a;z) \\ f(b;z) \end{pmatrix}, \quad Q(z) = \frac{1}{s(b;z)} \begin{pmatrix} -c(b;z) & 1 \\ 1 & -s'(b;z) \end{pmatrix},$$
(1.35)

and $Q(z)$ is the induced $\mathscr{Q}$-function.

A number of examples of boundary triples in problems concerning ordinary differential equations as well as their applications to scattering problems can be found e.g. in [18, 49].

The situation becomes much more complicated when dealing with elliptic differential equations on domains (or manifolds) with boundary. In this case the construction of a boundary triple involves certain information about the geometry of the domain, namely, the Dirichlet-to-Neumann map, see e.g. the recent works [16, 115] and the classical paper by Vishik [124], and the question on effective description of all self-adjoint boundary value problems for partial differential equations is still open, see the discussion in [54, 55] and historical comments in [75]; an explicit construction of boundary triples for the Laplacian in a bounded domain is presented in Example 5.5 in [115]. We remark that boundary triples provide only one possible choice of coordinates in the defect subspaces. Another possibility would be to use some generalization of boundary triples, for example, the so-called boundary relations resulting in unbounded Weyl functions [26, 48], but it seems that this technique is rather new and not developed enough for applications.

1.4.2 Singular perurbations

Here we discuss the construction of self-adjoint extensions in the context of the so-called singular perturbations; we follow in part the constriction of [114].

Let H^0 be a certain self-adjoint operator in a separable Hilbert space $\mathscr{H}$; its resolvent will be denoted by $R^0(z)$, $z \in \operatorname{res} H^0$. Denote by $\mathscr{H}_1$ the domain $\operatorname{dom} H_0$ equiped with the graph norm, $\|f\|_1^2 = \|H^0 f\|^2 + \|f\|^2$; clearly, $\mathscr{H}_1$ is a Hilbert space. Let $\mathscr{G}$ be another Hilbert space. Consider a bounded linear map $\tau : \mathscr{H}_1 \to \mathscr{G}$. We assume that τ is surjective and that $\ker \tau$ is dense in $\mathscr{H}$.

By definition, by a singular perturbation of H^0 supported by τ we mean any self-adjoint extension of the operator S which is the restriction of H^0 to $\operatorname{dom} S := \ker \tau$. Due to the above restrictions, S is a closed densely defined symmetric operator.

It is wortwhile to note that singular perturbations just provide another language for the general theory of self-adjoint extensions. Namely, let S by any closed densely defined symmetric operator with equal deficiency indices and H^0 be some its self-adjoint extension. Construct the space $\mathscr{H}_1$ as above. Clearly, $\mathscr{L} := \operatorname{dom} S$

is a closed subspace of $\mathscr{H}_1$, therefore, $\mathscr{H}_1 = \mathscr{L} \oplus \mathscr{L}^\perp$. Denoting $\mathscr{L}^\perp$ by $\mathscr{G}$ and the orthogonal projection from $\mathscr{H}_1$ to $\mathscr{L}^\perp$ by τ, we see the self-adoint extensions of S are exactly the singular perturbations of H^0 supported by τ. At the same time, knowing explicitly the map τ gives a possibility to construct a boundary triple for S.

Proposition 1.37. *The maps $\gamma(z)$, $\gamma(z) = \left(\tau R^0(\overline{z})\right)^*$, $z \in \operatorname{res} H^0$, form a Krein Γ-field for $(S, H^0, \mathscr{G})$.*

Proof. Note that the operator $A := \tau R^0(z) : \mathscr{H} \to \mathscr{G}$ is surjective, therefore, $\operatorname{ran} A^* = \ker A^\perp$. In other words,

$$\operatorname{ran} \gamma(z) = \ker \tau R^0(\overline{z})^\perp = \left\{ f \in \mathscr{H} : \tau R^0(\overline{z}) f = 0 \right\}^\perp$$
$$= \left\{ (H^0 - \overline{z})g : \tau g = 0 \right\}^\perp = \left\{ (S - \overline{z})g : g \in \operatorname{dom} S \right\}^\perp$$
$$= \operatorname{ran}(S - \overline{z})^\perp = \ker(S^* - z) =: \mathscr{N}_z. \quad (1.36)$$

Let us show that $\gamma(z)$ is an isomorphism of $\mathscr{G}$ and $\mathscr{N}_z$. First note that $\gamma(z)$ is bounded and, as we have shown above, surjective. Moreover, $\ker \gamma(z) = \operatorname{ran} A^\perp = \mathscr{G}^\perp = \{0\}$. Therefore, $\gamma(z) : \mathscr{G} \to \mathscr{N}_z$ has a bounded inverse defined everywhere by the closed graph theorem, and the condition (1.14a) is satisfied.

The condition (1.14b) is a corollary of the Hilbert resolvent identity. $\qquad\square$

Now one can construct a boundary triple for the operator S^*.

Proposition 1.38. *Take any $\zeta \in \operatorname{res} H^0$ and represent any $f \in \operatorname{dom} S^*$ in the form $f = f_\zeta + \gamma(\zeta)F$, $f_\zeta \in \operatorname{dom} H^0$, $F \in \mathscr{G}$, where γ is defined in proposition 1.37. Then $(\mathscr{G}, \Gamma_1, \Gamma_2)$, $\Gamma_1 f = F$, $\Gamma_2 f = \dfrac{1}{2}\tau\left(f_\zeta + f_{\overline{\zeta}}\right)$, is a boundary triple for S^*. The induced Γ-field is $\gamma(z)$, and the induced $\mathscr{Q}$-function $Q(z)$ has the form*

$$Q(z) = \frac{1}{2} z \tau R^0(z)\left(\gamma(\zeta) + \gamma(\overline{\zeta})\right) - \frac{1}{2}\tau R^0(z)\left(\zeta\gamma(\zeta) + \overline{\zeta}\gamma(\overline{\zeta})\right).$$

Proof. The major part follows from proposition 1.26. To obtain the formula for $Q(z)$ it is sufficient to see that for the function $f = \gamma(z)\varphi$, $\varphi \in \mathscr{G}$, one has $f_\zeta = \left(\gamma(z) - \gamma(\zeta)\right)\varphi$ and to use the property (1.14b). $\qquad\square$

Let us consider in greater detail a special type of the above construction, the so-called finite rank perturbations [8].

Let H^0 be as above. For $\alpha \geq 0$ denote by $\mathscr{H}_\alpha$ the domain of the operator $((H^0)^2 + 1)^{\alpha/2}$ equiped with the norm $\|f\|_\alpha = \left\|((H^0)^2 + 1)^{\alpha/2} f\right\|$. The space $\mathscr{H}_\alpha$ becomes a Hilbert space, and this notation is compatible with the above definition of $\mathscr{H}_1$, i.e. $\mathscr{H}_1$ is the domain of H^0 equiped with the graph norm, and $\mathscr{H}_0 = \mathscr{H}$.

Moreover, for $\alpha < 0$ we denote the completion of $\mathscr{H}$ with respect to the norm $\|f\|_\alpha = \|((H^0)^2 + 1)^{\alpha/2} f\|$. Clearly, $\mathscr{H}_\alpha \subset \mathscr{H}_\beta$ if $\alpha > \beta$.

Take $\psi_j \in \mathscr{H}_{-1}$, $j = 1, \ldots, n$. In many problems of mathematical physics one arrives at operators given by formal expressions of the form

$$H = H^0 + \sum_{j,k=1}^n \alpha_{jk} \langle \psi_j | \cdot \rangle \psi_k, \qquad (1.37)$$

where α_{jk} are certain numbers ("coupling constants"). This sum is not defined directly, as generically $\psi_j \notin \mathscr{H}$. At the same time, the operator H given by this expression is usually supposed to be self-adjoint (and then one has formally $\alpha_{jk} = \overline{\alpha_{kj}}$). Denote by S the restriction of H^0 to the functions $f \in \mathrm{dom}\, H^0$ with $\langle \psi_j | f \rangle = 0$ for all j; we additionally assume that ψ_j are linearly indepedent modulo $\mathscr{H}$ (otherwise S might become nondensely defined). Clearly, for any reasonable definition, the operators H^0 and H must coincide on the domain of S. Therefore, by definition, under an operator given by the right-hand side of (1.37) we understand the whole family of self-adjoint extensions of S. The boundary triple for S^* can be easily obtained using the above constructions if one set

$$\tau f := \begin{pmatrix} \langle \psi_1 | f \rangle \\ \ldots \\ \langle \psi_n | f \rangle \end{pmatrix} \in \mathbb{C}^n.$$

The corresponding Γ-field from proposition 1.37 takes the form

$$\gamma(z)\xi = \sum_{j=1}^n \xi_j h_j(z), \quad h_j(z) := R^0(z)\psi_j \in \mathscr{H}, \quad \xi = (\xi_1, \ldots \xi_n) \in \mathbb{C}^n,$$

and the boundary triples and the $\mathscr{Q}$-function are obtained using the formulas of proposition 1.38.

Unfortunately, the above construction has a severe disadvantage, namely, the role of the coefficients α_{jk} in (1.37) remains unclear. The definition of H using self-adjoint extensions involves self-adjoint linear relations in $\mathbb{C}^n$, and it is difficult to say what is the relationship between these two types of parameters. In some cases, if both H and H^0 have certain symmetries, this relationship can be found using a kind of renormalization technique [95, 97]. The situation becomes more simple if in the above construction one has $\psi_j \in \mathscr{H}_{-1/2}$ and H^0 is semibounded. In this case one can properly define H given by (1.37) using the corresponding quadratic form,

$$h(f,g) = h^0(f,g) + \sum_{j,k=1}^n \alpha_{jk} \langle f | \psi_j \rangle \langle \psi_k | g \rangle,$$

where h^0 is the quadratic form associated with H^0, see [89]. Also in this case one arrives at boundary triples and resolvent formulas. A very detailed analysis of rank-one perturbations of this kind with an extensive bibliography list is given in [121].

We also remark that one can deal with operator of the form (1.37) in the so-called supersingular case $\psi_j \notin \mathscr{H}_{-1}$; the corresponding operators H must be constructed then in an extended Hilbert or Pontryagin space, see e.g. [51, 95, 119] and references therein.

1.4.3 Point interactions on manifolds

Let X be a manifold of bounded geometry of dimension ν, $\nu \le 3$. Let $A = A_j dx^j$ be a 1-form on X, for simplicity we suppose here $A_j \in C^\infty(X)$. The functions A_j can be considered as the components of the vector potential of a magnetic field on X. On the other hand, A defines a connection ∇_A in the trivial line bundle $X \times \mathbb{C} \to X$, $\nabla_A u = du + iuA$; by $-\Delta_A = \nabla_A^* \nabla_A$ we denote the corresponding Bochner Laplacian. In addition, we consider a real-valued scalar potential U of an electric field on X. This potential will be assumed to satisfy the following conditions:

$$U_+ := \max(U, 0) \in L^{p_0}_{\text{loc}}(X), \quad U_- := \max(-U, 0) \in \sum_{i=1}^{n} L^{p_i}(X),$$

$$2 \le p_i \le \infty, \quad 0 \le i \le n;$$

we stress that p_i as well as n are not fixed and depend on U. The class of such potentials will be denoted by $\mathscr{P}(X)$. For the case $X = \mathbb{R}^n$ one can study Schrödinger operators with more general potentials from the Kato class [25, 122].

We denote by $H_{A,U}$ the operator acting on functions $\phi \in C_0^\infty(X)$ by the rule $H_{A,U}\phi = -\Delta_A \phi + U\phi$. This operator is essentially self-adjoint in $L^2(X)$ and semi-bounded below [36]; its closure will be also denoted by $H_{A,U}$. It is also known [36] that

$$\text{dom}\, H_{A,U} \subset C(X). \tag{1.38}$$

In what follows, the Green function $G_{A,U}(x, y; \zeta)$ of $H_{A,U}$, i.e. the integral kernel of the resolvent $R_{A,U}(\zeta) := (H_{A,U} - \zeta)^{-1}$, $\zeta \in \text{res}\, H_{A,U}$, will be of importance.

The most important its properties for us are the following ones:

for any $\zeta \in \text{res}\, H_{A,U}$, $G_{A,U}$ is continuous in $X \times X$ for $\nu = 1$ and in $X \times X \setminus \{(x,x), x \in X\}$ for $\nu = 2, 3$; $\tag{1.39a}$

for $\zeta \in \text{res}\, H^0$ and $y \in X$ one has $G_{A,U}(\cdot, y; \zeta) \in L^2(X)$; $\tag{1.39b}$

for any $f \in L^2(X)$ and $\zeta \in \text{res}\, H_{A,U}$, the function $x \mapsto \int_X G_{A,U}(x, y; \zeta) f(y) \, dy$ is continuous. $\tag{1.39c}$

We remark that for any $f \in \mathrm{dom}\, H_{A,U}$ and $\zeta \in \mathrm{res}\, H_{A,U}$ one has $f = R_{A,U}(\zeta)(H_{A,U} - \zeta)f$. Using the Green function we rewrite this as

$$f(x) = \int_X G_{A,U}(x,y;\zeta)(H_{A,U} - \zeta)f(y)\,dy \quad \text{a.e.;}$$

by (1.39c) and (1.38) the both sides are continuous functions of x, therefore, they coincide everywhere, i.e.

$$f(x) = \int_X G_{A,U}(x,y;\zeta)(H_{A,U} - \zeta)f(y)\,dy, \quad f \in \mathrm{dom}\, H_{A,U}, \text{ for all } x \in X. \quad (1.40)$$

Fix points $a_1,\ldots,a_n \in X$, $a_j \neq a_k$ if $j \neq k$, and denote by S the restriction of $H_{A,U}$ on the functions vanishing at all a_j, $j = 1,\ldots,n$. Clearly, due to (1.38) this restriction is well defined, and S is a closed densely defined symmetric operator. By definition, by a point perturbation of the operator $H_{A,U}$ supported by the points a_j, $j = 1,\ldots,n$, we mean any self-adjoint extension of S. Now we are actually in the situation of subsubsection 1.4.2. To simplify notation, we denote $H^0 := H_{A,U}$ and change respectively the indices for the resolvent and the Green function. Denote by τ the map

$$\tau : \mathrm{dom}\, H^0 \ni f \mapsto \begin{pmatrix} f(a_1) \\ \ldots \\ f(a_n) \end{pmatrix} \in \mathbb{C}^n.$$

By (1.40) and (1.39b), τ is bounded in the graph norm of H^0. Now let us use proposition 1.37. The map $\tau R^0(\overline{z})$ is of the form

$$f \mapsto \begin{pmatrix} \int_X G^0(a_1,y;\overline{z})f(y)dy \\ \ldots \\ \int_X G^0(a_n,y;\overline{z})f(y)dy \end{pmatrix}.$$

Calculating the adjoint operator and taking into account the identity $G^0(x,y;z) = \overline{G^0(y,x;\overline{z})}$ we arrive at

Lemma 1.39. *The map*

$$\gamma(\zeta) : \mathbb{C}^n \ni (\xi_1,\ldots,\xi_n) \mapsto \sum_{j=1}^n \xi_j G^0(\cdot,a_j;\zeta) \subset L^2(X) \quad (1.41)$$

is a Krein Γ-field for $(S,H^0,\mathbb{C}^n)$.

Let us construct a boundary triple corresponding to the problem. Use first corollary 1.27. Choose $\zeta \in \operatorname{res} H^0 \subset \mathbb{R}$; this is possible because H^0 is semi-bounded below. For any $f \in \operatorname{dom} S^*$ there are $F_j \in \mathbb{C}$ such that $f_\zeta := f - \sum_j F_j G^0(\cdot, a_j; \zeta) \in \operatorname{dom} H^0$. The numbers F_j are ζ-independent, and by corollary 1.27, the maps

$$\widetilde{\Gamma}_1 f := (F_1, \ldots, F_n), \quad \widetilde{\Gamma}_2 f = \big(f_\zeta(a_1), \ldots, f_\zeta(a_n)\big) \tag{1.42}$$

form a boundary triple for S^*. Nevertheless, such a construction is rarely used in practice due to its dependence on the energy parameter. We modifiy the above considerations using some information about the on-diagonal behavior of G^0.

Consider the case $\nu = 2$ or 3. As shown in [37], there exists a function $F(x,y)$ defined for $x \neq y$ such that for any $\zeta \in \operatorname{res} H^0$ there exists another function $G^0_{\mathrm{ren}}(x, y; \zeta)$ continuous in $X \times X$ such that

$$G^0(x, y; \zeta) = F(x, y) + G^0_{\mathrm{ren}}(x, y; \zeta), \tag{1.43}$$

and we additionally request $F(x,y) = \overline{F}(y,x)$. It is an important point that under some assumptions the function F can be chosen independent of the magnetic potential A_j and the scalar potential U. For example, if $\nu = 2$ one can always set $F(x,y) = \log \dfrac{1}{d(x,y)}$. In the case $\nu = 3$ the situation becomes more compli-cated. For example, for two scalar potentials U and V satisfying the above condi-tions one can take the same function F for the operators $H_{A,U}$ and $H_{A,V}$ provided $U - V \in L^q_{\mathrm{loc}}(X)$ for some $q > 3$. In pariticular, for any U satisying the above conditions and, additionally, $U \in L^q_{\mathrm{loc}}(X)$, for the operator $H_{0,U}$ one can always put $F(x,y) = \dfrac{1}{4\pi d(x,y)}$.

For the Schrödinger operator with a uniform magnetic field in $\mathbb{R}^3$, $H^0 = (i\nabla + A)^2$, where $\nabla \times A =: B$ is constant, one can put $F(x,y) := \dfrac{e^{iBxy/2}}{4\pi|x-y|}$. For a detailed discussion of on-diagonal singularities we refer to our paper [37].

Let us combine the representation (1.43) for the Green function and the equal-ity $\operatorname{dom} S^* = \operatorname{dom} H^0 + \mathcal{N}_\zeta$. Near each point a_j, any function $f \in \operatorname{dom} S^*$ has the following asymptotics:

$$f(x) = f_j + F_j F(x, a_j) + o(1), \quad f_j, F_j \in \mathbb{C}.$$

Proposition 1.40. *The triple $(\mathbb{C}^n, \Gamma_1, \Gamma_2)$ with $\Gamma_1 f = (F_1, \ldots, F_n) \in \mathbb{C}^n$ and $\Gamma_2 f = (f_1, \ldots, f_n) \in \mathbb{C}^n$ is a boundary triple for S^*.*

Proof. Let us fix some $\zeta \operatorname{res} H^0 \cap \mathbb{R}$. Comparing the maps Γ_j with the maps $\widetilde{\Gamma}_j$ from (1.42) one immediately see $\Gamma_1 \equiv \widetilde{\Gamma}_1$. Furthermore, $\Gamma_2 f = \widetilde{\Gamma}_2 f + B\widetilde{\Gamma}_1$, where

B is a $n \times n$ matrix,

$$B_{jk} = \begin{cases} G^0(a_j, a_k; \zeta) & \text{if } j \neq k, \\ G^0_{\text{ren}}(a_j, a_j; \zeta) & \text{otherwise.} \end{cases}$$

As $B = B^*$, it remains to use proposition 1.15. $\qquad\qquad\qquad\square$

Clearly, the map (1.41) is the Krein Γ-field induced by the boundary triple $(\mathbb{C}^n, \Gamma_1, \Gamma_2)$. The calculation of the corresponding $\mathscr{Q}$-function $Q(\zeta)$ gives

$$Q_{jk}(\zeta) = \begin{cases} G^0(a_j, a_k; \zeta) & \text{if } j \neq k, \\ G^0_{\text{ren}}(a_j, a_j; \zeta) & \text{otherwise.} \end{cases}$$

We note that the calculating of the $\mathscr{Q}$-function needs *a priori* the continuity of the Green function (otherwise the values of the Green function at single points would not be defined). A bibliography concerning the analysis of operators of the above type for particular Hamiltonians H^0 can be found e.g. in [6].

The above construction can generalized to the case of point perturbations supported by non-finite (but countable) sets provided some uniform discreteness, we refer to [63] for the general theory, to [7, 33, 69] for the analysis of periodic configurations, and to [22, 52, 77, 116] for multidimensional models with random interactions.

For analysis of interactions supported by submanifolds of higher dimension we refer to [19, 42, 43, 59, 60, 113] and references therein.

1.4.4 Direct sums and hybrid spaces

Assume that we have a countable family of closed linear operators S_α in some Hilbert spaces $\mathscr{H}_\alpha$, $\alpha \in \mathscr{A}$, having boundary triples $(\mathscr{G}^\alpha, \Gamma_1^\alpha, \Gamma_2^\alpha)$. Denote by H_α^0 the corresponding distinguished extensions, $H_\alpha^0 := S_\alpha|_{\ker \Gamma_1^\alpha}$. We impose some additional regularity conditions, namely, that:

- there exist constants a and b such that for any $\alpha \in \mathscr{A}$ and $f_\alpha \in \operatorname{dom} S_\alpha$ there holds $\|\Gamma_{1/2}^\alpha f_\alpha\| \leq a\|S_\alpha f_\alpha\| + b\|f_\alpha\|$,

- for any $(\xi_\alpha^{1/2}) \in \bigoplus_{\alpha \in \mathscr{A}} \mathscr{G}^\alpha$ there is $(f_\alpha) \in \bigoplus_{\alpha \in \mathscr{A}} \mathscr{H}_\alpha$, $f_\alpha \in \operatorname{dom} S_\alpha$, with $\Gamma_{1/2}^\alpha f_\alpha = \xi_\alpha^{1/2}$.

The above conditions are obviously satisfied if, for example, the operators S_α are copies of a finite set of operators, and the same holds for the boundary triples. Another situation where the conditions are satisfied, is provided by the operators

$S_\alpha = -\dfrac{d^2}{dx^2} + U_\alpha$ acting in $L^2[a_\alpha, b_\alpha]$ with the domains $H^2[a_\alpha, b_\alpha]$ provided that there are constants l_1, l_2, C such that $l_1 \le |a_\alpha - b_\alpha| < l_2$ and $\|U_\alpha\|_{L^2} < C$ and that the boundary triples are taken as in subsection 1.4.1, see [108] for details.

Under the above conditions, the operator $S := \bigoplus_{\alpha \in \mathscr{A}} S_\alpha$ acting in $\mathscr{H} := \bigoplus_{\alpha \in \mathscr{A}} \mathscr{H}_\alpha$ is closed and has a boundary triple $(\mathscr{G}, \Gamma_1, \Gamma_2)$,

$$\mathscr{G} := \bigoplus_{\alpha \in \mathscr{A}} \mathscr{G}_\alpha, \quad \Gamma_j := \bigoplus_{\alpha \in \mathscr{A}} \Gamma_j^\alpha, \quad j = 1, 2.$$

Moreover, the corresponding distinguished extension H^0 and the induced Krein maps γ and Q are also direct sums, i.e., at least

$$H^0 := \bigoplus_{\alpha \in \mathscr{A}} H_\alpha^0, \quad \gamma(z) = \bigoplus_{\alpha \in \mathscr{A}} \gamma^\alpha(z), \quad Q(z) = \bigoplus_{\alpha \in \mathscr{A}} Q^\alpha(z).$$

Note that $\gamma(z)$ and $Q(z)$ are defined only for $z \notin \operatorname{spec} H^0 \equiv \overline{\bigcup_{\alpha \in \mathscr{A}} \operatorname{spec} H_\alpha^0}$. Let us show how this abstract construction can be used to define Schrödinger operators on hybrid spaces, i.e. on configurations consisting of pieces of different dimensions.

Let M_α, $\alpha \in \mathscr{A}$, be a countable family of manifolds as in subsubsection 1.4.3. Fix several points $m_{\alpha j} \in \mathscr{M}_\alpha$, $j = 1, \dots, n_\alpha$. We interpret these points as points of glueing. More precisely, we consider a matrix T with the entries $T_{(\alpha j)(\beta k)}$ such that $T_{(\alpha j)(\beta k)} = 1$ if the point $m_{\alpha j}$ is identified with $m_{\beta k}$ (i.e. point $m_{\alpha j}$ of M_α is glued to the point $m_{\beta k}$ of M_β), and $T_{(\alpha j)(\beta k)} = 0$ otherwise. The obtained topological space is not a manifold as it has singularities at the points of glueing; we will refer it to as a *hybrid manifold*. Our aim is to show how to define a Schrödinger operator in such a structure.

On of the manifolds M_α consider Schrödinger operators H_α as in subsubsection 1.4.3. To satisfy the above regularity conditions we request that these operators are copies of a certain finite family. For $\alpha \in \mathscr{A}$ denote by S_α the restriction of H_α to the functions vanishing at all the points $m_{\alpha j}$ and construct a boudary triple $(\mathbb{C}^{m_\alpha}, \Gamma_{\alpha 1}, \Gamma_{\alpha 2})$ for S_α^* as in in subsubsection 1.4.3. Clearly, as a boundary triple for the operator S^*, $S := \bigoplus_{\alpha \in \mathscr{A}} S_\alpha$, in the space $L^2(M) := \bigoplus_{\alpha \in \mathscr{A}} L^2(M_\alpha)$ one take $(\mathscr{G}, \Gamma_1, \Gamma_2)$ with $\mathscr{G} := \bigoplus_{\alpha \in \mathscr{A}} \mathbb{C}^{n_\alpha}$, $\Gamma_j(f_\alpha) = (\Gamma_{\alpha j} f_\alpha)$, $j = 1, 2$. Under a Schrödinger operator on $L^2(M)$ one can mean any self-adjoint extension of S. To take into account the way how the manifolds are glued with each other, one should restrict the class of possible boundary conditions. A reasonable idea would be to consider boundary conditions of the form $A\Gamma_1 = B\Gamma_2$ such that $A_{(\alpha j)(\beta k)} = B_{(\alpha j)(\beta k)} = 0$ if $T_{(\alpha j)(\beta k)} = 0$, i.e. assuming that each boundary condition involves only points glued to each other.

The analysis of generic Schrödinger operators on hybrid manifolds is hardly possible, as even Schrödinger operators on a single manifold do not admit the

complete analysis. One can say some more about particular configuration, for example, if one has only finitely many pieces M_α and they all are compact [57]. Some additional information can be obtained for periodic configurations [30, 32].

One can extend the above construction by combining operators from subsection 1.4.1 and 1.4.3; in this way one arrive at a space with consists of manifolds connected with each other through one-dimensional segments.

One can also take a direct sum of operators from subsubsection 1.4.1 to define a Schrödinger operator on a configuration consisting of segments and halflines connected with each other; such operators are usually referred to as *quantum graphs*, and their analysis becomes very popular in the last decades, see e.g. [21] for the review and recent developments.

2 Classification of spectra of self-adjoint operators

2.1 Classification of measures

Here we recall briefly some concepts of the measure theory.

Let $\mathscr{B}$ be the set of all the Borel subsets of a locally compact separable metric space X. A mapping $\mu : \mathscr{B} \to [0, +\infty]$ is called a *positive Borel measure* on X if it is σ-additive (i.e. $\mu(\bigcup_k B_k) = \sum_k \mu(B_k)$ for every countable family (B_k) of mutually not-intersecting sets from $\mathscr{B}$) and has the following regularity properties:

- $\mu(K) < \infty$ for every compact $K \subset X$;

- for every $B \in \mathscr{B}$ there holds $\mu(B) = \sup\{\mu(K) : K \subset B, K \text{ is compact}\} = \inf\{\mu(G) : G \supset B, G \text{ is open}\}$.

A complex valued Borel measure on X is a σ-additive mapping $\mu : \mathscr{B} \to \mathbb{C}$ such that the variation $|\mu|$ of μ defined on $\mathscr{B}$ by

$$|\mu|(B) = \sup \sum |\mu(B_k)|,$$

where the supremum is taken over all finite families (B_k) of mutually non-intersecting sets B_k from $\mathscr{B}$ such that $\bigcup B_k \subset B$, is a Borel measure. For a positive measure μ one has $|\mu| = \mu$. If $|\mu|(X) < \infty$, then μ is called *finite* (or *bounded*) and $|\mu|(X)$ is denoted also by $\|\mu\|$. We will denote by $\mathscr{M}(X)$ (respectively, by $\mathscr{M}^+(X)$) the set of all complex Borel measures (respectively, the set of all positive Borel measures) on X; if $X = \mathbb{R}$ we write simply $\mathscr{M}$ and $\mathscr{M}^+$. It is clear that $\mathscr{M}(X)$ is a complex vector space (even a complex vector lattice) and the subset $\mathscr{M}^{\mathrm{b}}(X)$ of all bounded measures from $\mathscr{M}(X)$ is a vector subspace of $\mathscr{M}(X)$ which is a Banach space with respect to the norm $\|\mu\|$.

Ona says that a measure μ is *concentrated* on a Borel set $S \in \mathcal{B}$, if $\mu(B) = \mu(B \cap S)$ for all $B \in \mathcal{B}$. Let μ_1 and μ_2 be two measures; they are called *disjoint* or *mutually singular*, if there exists two disjoint Borel set S_1 and S_2 such that μ_j is concentrated on S_j $(j = 1, 2)$; we will write $\mu_1 \perp \mu_2$ if μ_1 and μ_2 are disjoint. The measure μ_1 is said to be *subordinated* to μ_2 (or *absolutely continuous with respect to μ_2*) if every $|\mu_2|$-negligible Borel set is simultaneously $|\mu_1|$-negligible. According to the Radon–Nikodym theorem, the following assertions are equivalent: (1) μ_1 is subordinated to μ_2; (2) there exists a Borel function f such that $\mu_1 = f\mu_2$ (in this case $f \in L^1_{loc}(X, \mu_2)$ and f is called the *Radon–Nikodym derivative* of μ_1 with respect to μ_2). If μ_1 is subordinated to μ_2 and simultaneously μ_2 is subordinated to μ_1 (i.e., if μ_1 and μ_2 have the same negligible Borel sets), then μ_1 and μ_2 are called *equivalent* (in symbols: $\mu_1 \sim \mu_2$). For a subset $M \subset \mathcal{M}(X)$ we denote $M^\perp = \{\mu \in \mathcal{M}(X) : \mu \perp \nu \ \forall \nu \in M\}$; $M^\perp$ is a vector subspace of $\mathcal{M}(X)$. A *subspace* $M \subset \mathcal{M}(X)$ is called a *band* (or a *component*) in $\mathcal{M}(X)$, if $M = M^{\perp\perp}$. For every subset $L \in \mathcal{M}(X)$ the set $L^\perp$ is a band; the band $L^{\perp\perp}$ is called the *band generated by L*. In particular, if $\mu \in \mathcal{M}(X)$, then the band $\{\mu\}^{\perp\perp}$ consists of all ν which are subordinated to μ. Moreover, μ_1 is subordinated to μ_2 if and only if $\{\mu_1\}^{\perp\perp} \subset \{\mu_2\}^{\perp\perp}$; in particular, $\mu_1 \sim \mu_2$ if and only if $\{\mu_1\}^{\perp\perp} = \{\mu_2\}^{\perp\perp}$. The bands M and N are called *disjoint*, if $\mu \perp \nu$ for every pair $\mu \in M$ and $\nu \in N$.

The family $(L_\xi)_{\xi \in \Xi}$ of bands in $\mathcal{M}(X)$ such that $\mu \in \left(\bigcup_{\xi \in \Xi} L_\xi \right)^\perp$ implies $\mu = 0$ is called *complete*. Let a complete family of mutually disjoint bands L_ξ, $\xi \in \Xi$, is given. Then for every $\mu \in \mathcal{M}(X)$, $\mu \geq 0$, there exists a unique family $(\mu_\xi)_{\xi \in \Xi}$, $\mu_\xi \in L_\xi$, such that $\mu = \sup_{\xi \in \Xi} \mu_\xi$, where the supremum is taken in the vector lattice $\mathcal{M}(X)$; μ_ξ is called the *component* of μ in L_ξ. If, in addition, the family (L_ξ) is finite, then $\mathcal{M}(X)$ is the direct sum of (L_ξ) and μ is the sum of its components μ_ξ.

In particular, if L is a band, then the pair $(L, L^\perp)$ is a complete family of mutually disjoint bands; the component of a measure μ in L coincides in this case with the projection of μ onto L parallel to $L^\perp$ and denoted by μ^L. The measure μ^L is completely characterized by the following two properties:

- $\mu^L \in L$;

- $(\mu - \mu_L) \perp L$.

A Borel measure μ is called a *point* or *atomic* measure, if it is concentrated on a countable subset $S \subset X$. A point $s \in S$ such that $\mu(\{s\}) \neq 0$ is called an atom for μ. For every set $B \in \mathcal{B}$ there holds

$$\mu(B) = \sum_{s \in B \cap S} \mu(\{s\}).$$

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The set of all complex point Borel measures on X we will denote by $\mathcal{M}_p(X)$, this is a band in $\mathcal{M}(X)$.

A Borel measure μ is called a *continuous* measure, if $\mu(\{s\}) = 0$ for every $s \in X$. The set of all continuous Borel measures on X we will denote by $\mathcal{M}_c(X)$. It is clear that $\mathcal{M}_c^{\perp}(X) = \mathcal{M}_p(X)$, $\mathcal{M}_p^{\perp}(X) = \mathcal{M}_c(X)$, and $\mathcal{M}(X)$ is the direct sum of the bands $\mathcal{M}_p(X)$ and $\mathcal{M}_c(X)$.

Let now X be a locally compact separable metric group with the continuous Haar measure. We fix the left Haar measure λ; if X is a compact space, we choose λ to be normalized, in the case $X = \mathbb{R}$ we choose λ to be the Lebesgue measure. A measure μ on X is called *absolutely continuous*, if it is subordinated to λ and *singular*, if it is disjoint to λ (it is clear that these definitions are independent on the particular choice of λ). The set of all absolutely continuous Borel measures on X (respectively, the set of all singular Borel measures on X) will be denoted by $\mathcal{M}_{ac}(X)$ (respectively, by $\mathcal{M}_s(X)$). In particular, $\mathcal{M}_p(X) \subset \mathcal{M}_s(X)$. It is clear that $\mathcal{M}_s^{\perp}(X) = \mathcal{M}_{ac}(X)$, $\mathcal{M}_{ac}^{\perp}(X) = \mathcal{M}_s(X)$, and $\mathcal{M}(X)$ is the direct sum of the bands $\mathcal{M}_{ac}(X)$ and $\mathcal{M}_s(X)$.

A Borel measure μ on X is called a *singular continuous* measure, if it is simultaneously continuous and singular. The set of all singular continuous Borel measures on X we will denote by $\mathcal{M}_{sc}(X)$; this is a band in $\mathcal{M}(X)$. By definition $\mu \in \mathcal{M}_{sc}$ if and only if μ is concentrated on a Borel set of zero Haar measure and $\mu(S) = 0$ for every countable set S.

According to the *Lebesgue decomposition theorem* each Borel measure μ on the group X is decomposable in a unique way into the sum

$$\mu = \mu^p + \mu^{ac} + \mu^{sc},$$

where $\mu^p \in \mathcal{M}_p(X)$, $\mu^{ac} \in \mathcal{M}_{ac}(X)$, $\mu^{sc} \in \mathcal{M}_{sc}(X)$. We will denote also $\mu^c = \mu^{ac} + \mu^{sc}$ and $\mu^s = \mu^p + \mu^{sc}$. It is clear that $\mu^c \in \mathcal{M}_c(X)$, $\mu^s \in \mathcal{M}_s(X)$.

2.2 Spectral types and spectral measures

In this section, A denotes a self-adjoint operator in a Hilbert space $\mathcal{H}$, $\mathrm{res}\,A$ is the resolvent set of A, $\mathrm{spec}\,A := \mathbb{C} \setminus \mathrm{res}\,A$ is the spectrum of A. For $z \in \mathrm{res}\,A$ we denote $R(z;A) := (A - z)^{-1}$ (the resolvent of A).

The first classification of spectra is related to the stability under compact perturbations of A. By definition, the *discrete* spectrum of A (it is denoted by $\mathrm{spec}_{dis}\,A$) consists of all *isolated* eigenvalues of *finite* multiplicity, and the *essential* spectrum of A, $\mathrm{spec}_{ess}\,A$, is the complement of the discrete spectrum in the whole spectrum: $\mathrm{spec}_{ess}\,A = \mathrm{spec}\,A \setminus \mathrm{spec}_{dis}\,A$. By the famous Weyl perturbation theorem, for a point $x_0 \in \mathrm{spec}\,A$ the following assertions are equivalent

- $\zeta \in \mathrm{spec}_{ess}\,A$,

- for every compact operator K in $\mathscr{H}$ there holds $\zeta \in \mathrm{spec}_{\mathrm{ess}}(A+K)$.

The second classification is related to the transport and scattering properties of a quantum mechanical system with the Hamiltonian $H = A$. For $\Omega \in \mathscr{B}$ denote $P_\Omega(A) = \chi_\Omega(A)$, where χ_Ω is the indicator function of the subset $\Omega \subset \mathbb{R}$; $P_\Omega(A)$ is the spectral projector for A on the subset Ω. The mapping $\mathscr{B} \ni \Omega \mapsto P_\Omega(A)$ is called the projection valued measure associated with A (the resolution of identity). For every pair $\varphi, \psi \in \mathscr{H}$, the mapping

$$\mathscr{B} \ni \Omega \mapsto \langle \varphi | P_\Omega(A)\psi \rangle = \langle P_\Omega(A)\varphi | P_\Omega(A)\psi \rangle$$

is a complex Borel measure on the real line $\mathbb{R}$ which is called the *spectral measure* associated with the triple (A, φ, ψ) and denoted by $\mu_{\varphi,\psi}$ (or more precisely, by $\mu_{\varphi,\psi}(\cdot; A)$). If $\varphi = \psi$, then $\mu_\varphi \equiv \mu_{\varphi,\varphi}$ is a bounded positive Borel measure on $\mathbb{R}$,

$$\mathscr{B} \ni \Omega \mapsto \langle \varphi | P_\Omega(A)\varphi \rangle = \| P_\Omega(A)\varphi \|^2,$$

with the norm $\|\mu_\varphi\| = \|\varphi\|^2$. Therefore, $\mu_{\varphi,\psi}$ is bounded and

$$|\mu_{\varphi,\psi}|(\Omega) \leq \big[\mu_\varphi(\Omega)\mu_\psi(\Omega) \big]^{1/2}.$$

Moreover, $\mathrm{supp}\, \mu_{\varphi,\psi} \subset \mathrm{spec}\, A$.

According to the Riesz–Markov theorem, for a bounded complex Borel measure μ on $\mathbb{R}$ the following three conditions are equivalent:

- $\mu = \mu_{\varphi,\psi}$ for some $\varphi, \psi \in \mathscr{H}$;

- for every continuous function f on $\mathbb{R}$ with compact support

$$\langle \varphi | f(A)\psi \rangle = \int_\mathbb{R} f(x)\, d\mu(x);$$

- for every bounded Borel function f on $\mathbb{R}$

$$\langle \varphi | f(A)\psi \rangle = \int_\mathbb{R} f(x)\, d\mu(x).$$

The following proposition is obvious.

Proposition 2.1. *For a Borel subset $\Omega \subset \mathbb{R}$ the following assertions hold:*

(1) $\mu_\varphi(\Omega) = 0$ *if and only if* $P_\Omega \varphi = 0$.

(2) μ_φ *is concentrated on* Ω *if and only if* $P_\Omega \varphi = \varphi$.

Proposition 2.2. *The following assertions take place.*

(1) $\mu_{\varphi,\psi}$ and $\mu_{\varphi+\psi}$ are subordinated to $\mu_\varphi + \mu_\psi$;

(2) $\mu_{a\varphi} = |a|^2 \mu_\varphi$ for every $a \in \mathbb{C}$;

(3) if $\mu_\varphi \perp \mu_\psi$, then $\varphi \perp \psi$;

(4) if $\mu_\varphi \perp \mu_\psi$, and $B = f(A)$ where f is a bounded Borel function, then $\mu_{B\varphi} \perp \mu_\psi$;

(5) if $\mu_{\varphi_n} \perp \mu_\psi$ for a sequence φ_n from $\mathcal{H}$, and $\varphi_n \to \varphi$ in $\mathcal{H}$, then $\mu_\varphi \perp \mu_\psi$.

Proof. (1) For $B \in \mathcal{B}$ we have:

$$|\mu_{\varphi,\psi}|(B) \leq \|P_B(\varphi)\| \, \|P_B(\psi)\|,$$

$$\left[\mu_{\varphi+\psi}(B)\right]^{1/2} = \|P_B(\varphi+\psi)\| \leq \|P_B(\varphi)\| + \|P_B(\psi)\|,$$

hence $|\mu_{\varphi,\psi}|(B) = \mu_{\varphi+\psi}(B) = 0$, if $\mu_{\varphi+\psi}(B) = 0$.

(2) Trivial.

(3) Let $S, T \in \mathcal{B}$, $S \cap T = \emptyset$, μ_φ be concentrated on S and μ_ψ be concentrated on T. Then, according to proposition 2.1, $\langle \varphi, \psi \rangle = \langle P_S \varphi, P_T \psi \rangle = \langle \varphi, P_S P_T \psi \rangle = 0$.

(4) Let S and T be as in item (3). Then $P_S \varphi = \varphi$, $P_T \psi = \psi$. Hence $P_S f(A) \varphi = f(A) P_S \varphi = f(A) \varphi$ and we can refer to proposition 2.1

(5) Let $S_n, T_n \in \mathcal{B}$, $S_n \cap T_n = \emptyset$, μ_{φ_n} be concentrated on S_n and μ_ψ be concentrated on T_n. Set $T = \bigcap T_n$, $S = \mathbb{R} \setminus T$. Then μ_{φ_n} is concentrated on S for every n and μ_ψ is concentrated on T. By proposition 2.1, $P_S \varphi_n = \varphi_n$, $P_T \psi = \psi$. As a result, we have $P_S \varphi = \varphi$, hence $\mu_\varphi \perp \mu_\psi$ by proposition 2.1. $\square$

Let L be a band in $\mathcal{M}$. Denote $\mathcal{H}_L \equiv \{\psi \in \mathcal{H} : \mu_\psi \in L\}$. Then by proposition 2.2 $\mathcal{H}_L$ is a closed A-invariant subspace of $\mathcal{H}$. Moreover, let $(L_\xi)_{\xi \in \Xi}$ be a complete family of bands in $\mathcal{M}$. Then $\mathcal{H}$ is the closure of the linear span of the family of closed A-invariant subspaces $\mathcal{H}_{L_\xi}$. If, in addition, L_ξ are mutually disjoint then $\mathcal{H}$ is the orthogonal sum of $\mathcal{H}_{L_\xi}$. In particular, $\mathcal{H}_L^\perp = \mathcal{H}_{L^\perp}$. Moreover, the following proposition is true.

Proposition 2.3. *Let $\varphi \in \mathcal{H}$ and φ_L is the orthogonal projection of φ onto $\mathcal{H}_L$. Then*

(1) $\mu_\varphi - \mu_{\varphi_L} \geq 0$ and is subordinated to $\mu_{\varphi-\varphi_L}$;

(2) $\mu_{\varphi_L} = \mu_\varphi^L$.

Proof. (1) First of all we show that $\mu_\varphi - \mu_{\varphi_L} \geq 0$. Let $B \in \mathscr{B}$, then $(\mu_\varphi - \mu_{\varphi_L})(B) = \|P_B\varphi\|^2 - \|P_B P_{\mathscr{H}_L}\varphi\|^2$. Since $\mathscr{H}_L$ is A-invariant, $P_B P_{\mathscr{H}_L} = P_{\mathscr{H}_L} P_B$, therefore $(\mu_\varphi - \mu_{\varphi_L})(B) = \|P_B\varphi\|^2 - \|P_{\mathscr{H}_L} P_B\varphi\|^2 \geq 0$.

Further we have for $B \in \mathscr{B}$

$$
\begin{aligned}
(\mu_\varphi - \mu_{\varphi_L})(B) & \\
= \|P_B\varphi\|^2 - \|P_B\varphi_L\|^2 &= (\|P_B\varphi\| + \|P_B\varphi_L\|)(\|P_B\varphi\| - \|P_B\varphi_L\|) \\
&\leq 2\|\varphi\|\|P_B(\varphi - \varphi_L)\| = 2\|\varphi\| \left[\mu_{\varphi - \varphi_L}(B)\right]^{1/2},
\end{aligned}
$$

and the proof of the item is complete.

(2) $\mu_{\varphi_L} \in L$, and according to item (1) $\mu_\varphi - \mu_{\varphi_L} \in L^\perp$. $\qquad\square$

Since $\mathscr{H}_L$ is A invariant, the restriction of A to $\mathscr{H}_L$ is a self-adjoint operator in $\mathscr{H}_L$. The spectrum of this restriction is denoted by $\mathrm{spec}_L A$ and is called *L-part* of the spectrum of A.

It is clear that for a point $x_0 \in \mathbb{R}$ the following assertions are equivalent:

- $x_0 \in \mathrm{spec} A$;

- for any $\varepsilon > 0$ there exists $\varphi \in \mathscr{H}$ such that $\mu_\varphi(x_0 - \varepsilon, x_0 - \varepsilon) > 0$.

Therefore, we have

Proposition 2.4. *The following assertions are equivalent:*

- $x_0 \in \mathrm{spec}_L A$;

- *for any $\varepsilon > 0$ there exists $\varphi \in \mathscr{H}$ with $\mu_\varphi^L(x_0 - \varepsilon, x_0 - \varepsilon) > 0$;*

- *for any $\varepsilon > 0$ there exists $\varphi \in \mathscr{H}_L$ with $\mu_\varphi(x_0 - \varepsilon, x_0 - \varepsilon) > 0$.*

Let $(L_\xi)_{\xi \in \Xi}$ be a complete family of mutually disjoint bands in $\mathscr{M}$. Then

$$
\mathrm{spec} A = \overline{\bigcup_{\xi \in \Xi} \mathrm{spec}_{L_\xi} A}.
$$

Let L be a band in $\mathscr{M}$, $N = L^\perp$ and $\Omega \in \mathscr{B}$. If $B \cap \mathrm{spec}_M A = \emptyset$, then we say that A has only L-spectrum on Ω (or the spectrum of A on Ω is purely L).

Denote now $\mathscr{H}_j$, where $j \in \{\mathrm{p}, \mathrm{ac}, \mathrm{sc}, \mathrm{s}, \mathrm{c}\}$, the subspace $\mathscr{H} \equiv \mathscr{H}_{\mathscr{M}_j}$. Then the spectrum of the restriction of A to $\mathscr{H}_j$ is denoted $\mathrm{spec}_j A$. In particular,

- $\mathscr{H} = \mathscr{H}_\mathrm{p} \oplus \mathscr{H}_\mathrm{ac} \oplus \mathscr{H}_\mathrm{sc}$, therefore $\mathrm{spec} A = \mathrm{spec}_\mathrm{p} A \cup \mathrm{spec}_\mathrm{ac} A \cup \mathrm{spec}_\mathrm{sc} A$. The part $\mathrm{spec}_\mathrm{p} A$ is called the *point* spectrum of A, $\mathrm{spec}_\mathrm{ac} A$ is called the *absolutely continuous* spectrum of A and $\mathrm{spec}_\mathrm{sc} A$ is called the *singular continuous* spectrum of A.

- $\mathcal{H} = \mathcal{H}_{\mathrm{p}} \oplus \mathcal{H}_{\mathrm{c}}$, therefore $\operatorname{spec} A = \operatorname{spec}_{\mathrm{p}} A \cup \operatorname{spec}_{\mathrm{c}} A$. The part $\operatorname{spec}_{\mathrm{c}} A$ is called the *continuous* spectrum of A.

- $\mathcal{H} = \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{s}}$, therefore $\operatorname{spec} A = \operatorname{spec}_{\mathrm{ac}} A \cup \operatorname{spec}_{\mathrm{s}} A$. The part $\operatorname{spec}_{\mathrm{s}} A$ is called the *singular* spectrum of A.

Consider the point part of the spectrum in detail. The set of all eigenvalues of A is denoted by $\operatorname{spec}_{\mathrm{pp}} A$ and is called *pure point* spectrum of A. In particular, for a point $x_0 \in \mathbb{R}$ the following assertions are equivalent:

- $x_0 \in \operatorname{spec}_{\mathrm{pp}} A$;

- $\mu_\varphi(\{x_0\}) > 0$ for some $\varphi \in \mathcal{H}$.

Proposition 2.5. *Let δ_a, where $a \in \mathbb{R}$, be the Dirac measure concentrated on a. Then for $a \in \mathbb{R}$ and $\varphi \in \mathcal{H}$ the following conditions are equivalent*

(1) $P_{\{a\}} \varphi = \varphi$;

(2) $\mu_\varphi = \|\varphi\|^2 \delta_a$;

(3) $A\varphi = a\varphi$.

Proof. $(1) \Rightarrow (2)$. For $\Omega \in \mathcal{B}$ we have $\mu_\varphi(\Omega) = \|P_\Omega \varphi\|^2 = \|P_\Omega P_{\{a\}} \varphi\|^2$. Therefore, $\mu_\varphi(\Omega) = \|\varphi\|^2$, if $a \in \Omega$ and $\mu_\varphi(\Omega) = 0$ otherwise.

$(2) \Rightarrow (3)$. We have for a $z \in \operatorname{res}(A)$

$$\langle \varphi | R(z;A)\varphi \rangle = \int\limits_{\mathbb{R}} \frac{d\mu_\varphi(x)}{x-z} = \frac{\|\varphi\|^2}{a-z},$$

hence, by polarization, $R(z;A)\varphi = (a-z)^{-1}\varphi$.

$(3) \Rightarrow (1)$. Indeed, $P_{\{a\}} = \chi_{\{a\}}(A)$ and $\chi_{\{a\}}(a) = 1$. $\square$

As a corollary we have that if a is an atom for a spectral measure μ_ψ, then $a \in \operatorname{spec}_{\mathrm{pp}} A$. Indeed, if $\mu_\psi(\{a\}) > 0$, then $\varphi = P_{\{a\}} \neq 0$. On the other hand, $P_{\{a\}}\varphi = \varphi$.

Proposition 2.6. *$\mathcal{H}_{\mathrm{p}}$ is the orthogonal direct sum $\mathcal{H}_{\mathrm{pp}}$ of the eigensubspaces of A, and $\operatorname{spec}_{\mathrm{p}} A = \overline{\operatorname{spec}_{\mathrm{pp}} A}$.*

Proof. It is clear that $\mathcal{H}_{\mathrm{pp}} \subset \mathcal{H}_{\mathrm{p}}$. To show that $\mathcal{H}_{\mathrm{pp}} \supset \mathcal{H}_{\mathrm{p}}$ it is sufficient to prove that if $\psi \perp \mathcal{H}_{\mathrm{pp}}$, then μ_ψ has no atoms. Suppose that $\psi \perp \mathcal{H}_{\mathrm{pp}}$ but $\mu_\psi(\{a\}) > 0$. Then $\varphi = P_{\{a\}} \psi \neq 0$. Further, $\varphi = P_{\{a\}}\varphi$, therefore $\varphi \in \mathcal{H}_{\mathrm{pp}}$. On the other hand $\langle \psi, \varphi \rangle = \langle \psi, P_{\{a\}} \psi \rangle = \mu_\psi(\{a\}) > 0$.

It is clear that $\operatorname{spec}_{\mathrm{pp}} A \subset \operatorname{spec}_{\mathrm{p}} A$. Suppose that $a \in \operatorname{spec}_{\mathrm{p}} A$. Take $\varepsilon > 0$, then $\mu_\psi(a - \varepsilon, a + \varepsilon) > 0$ for some $\psi \in \mathcal{H}_{\mathrm{p}}$. Hence, there is an atom s for μ_ψ such that $s \in (a - \varepsilon, a + \varepsilon)$. It remains to remark that $s \in \operatorname{spec}_{\mathrm{pp}} A$. $\square$

The considered classifications of spectra are related as follows.

- $\mathrm{spec}_{\mathrm{dis}} A \subset \mathrm{spec}_{\mathrm{pp}} A$;

- $\mathrm{spec}_{\mathrm{ess}} A$ is the union of the following three sets:

  (1) $\mathrm{spec}_{\mathrm{c}} A$,

  (2) $\{x \in \mathbb{R} : x \text{ is a limiting point of } \mathrm{spec}_{\mathrm{pp}} A\}$,

  (3) $\{x \in \mathrm{spec}_{\mathrm{pp}} A : x \text{ is of infinite multiplicity}\}$.

2.3 Spectral projections

Let $x, y \in \mathbb{R}$. In what follows we will use often the identities

$$
\begin{aligned}
\mathrm{Im} \left\langle \varphi \big| R(x+iy;A)\varphi \right\rangle &= \frac{1}{2i} \left[\langle \varphi | R(x+iy;A)\varphi \rangle - \langle R(x+iy;A)\varphi | \varphi \rangle \right] \\
&= \frac{1}{2i} \left\langle \varphi \big| \left[R(x+iy;A) - R(x-iy;A) \right] \varphi \right\rangle \\
&= y \langle \varphi | R(x-iy;A)R(x+iy;A) \rbrack \varphi \rangle \\
&= y \| R(x+iy;A)\varphi \|^2 .
\end{aligned}
\tag{2.1}
$$

The following Stone formulas for spectral projections will be very useful, cf. Theorem 42 in [84]. Let $-\infty < a < b < +\infty$ and $\varphi \in \mathcal{H}$, then

$$
\begin{aligned}
\frac{1}{2} \left[P_{[a,b]} \varphi + P_{(a,b)} \varphi \right] &= \lim_{y \to +0} \frac{1}{2\pi i} \int_a^b \left[R(x+iy;A) - R(x-iy;A) \right] \varphi \, dx \\
&= \lim_{y \to +0} \frac{1}{\pi} \int_a^b \left[\mathrm{Im}\, R(x+iy;A) \right] \varphi \, dx \\
&= \lim_{y \to +0} \frac{y}{\pi} \int_a^b R(x-iy;A)R(x+iy;A)\varphi \, dx .
\end{aligned}
\tag{2.2}
$$

Since $\mu_\varphi(\Omega) = \langle \varphi | P_\Omega(A)\varphi \rangle = \| P_\Omega(A)\varphi \|^2$, we have for $a, b \in \mathbb{R} \setminus \mathrm{spec}_{\mathrm{pp}}(A)$

$$
\begin{aligned}
\mu_\varphi((a,b)) = \mu_\varphi([a,b]) &= \lim_{y \to +0} \frac{1}{\pi} \int_a^b \mathrm{Im} \langle \varphi | R(x+iy;A)\varphi \rangle \, dx \\
&= \lim_{y \to +0} \frac{1}{\pi} \mathrm{Im} \int_a^b \langle \varphi | R(x+iy;A)\varphi \rangle \, dx \\
&= \lim_{y \to +0} \frac{y}{\pi} \int_a^b \| R(x+iy;A)\varphi \|^2 \, dx .
\end{aligned}
\tag{2.3}
$$

If $a \in \mathbb{R}$ and $\varphi \in \mathscr{H}$, then $P_{\{a\}}(A)\varphi = -i \lim\limits_{y\to+0} yR(a+iy;A)\varphi$, therefore

$$\mu_\varphi(\{a\}) = \|P_{\{a\}}(A)\varphi\|^2 = \lim\limits_{y\to+0} y^2 \|R(a+iy;A)\varphi\|^2.$$

The following statement is known [11, 84]

Theorem 2.7. *Let $\varphi \in \mathscr{H}$. For Lebesgue a.e. $x \in \mathbb{R}$ there exists the limit*

$$\langle \varphi|R(x+i0;A)\varphi\rangle := \lim\limits_{y\to0+} \langle \varphi|R(x+iy;A)\varphi\rangle;$$

this limit is is finite and non-zero a.e. and, additionally, using (2.1),

(1) $\mu_\varphi^{\mathrm{ac}} = \pi^{-1} F_\varphi \, dx$, *where*

$$F_\varphi(x) = \mathrm{Im}\,\langle \varphi|R(x+i0;A)\varphi\rangle = \lim\limits_{y\to0+} y\|R(x+iy)\varphi\|^2.$$

(2) μ_φ^{s} *is concentrated on the set $\{x \in \mathbb{R} : \mathrm{Im}\,\langle \varphi|R(x+i0;A)\varphi\rangle = \infty\}$.*

Additionally, for $-\infty < a \le b < +\infty$ one has:

(3) $\mu_\varphi^{\mathrm{ac}}([a,b]) = 0$ *if and only if for some p, $0 < p < 1$,*

$$\lim\limits_{y\to0+} \int_a^b [\mathrm{Im}\,\langle \varphi|R(x+iy;A)\varphi\rangle]^p \, dx = 0.$$

(4) Assume that for some p, $1 < p \le \infty$ one has

$$\sup\{\|\mathrm{Im}\,\langle\varphi|R(\cdot+iy;A)\varphi\rangle\|_p : 0 < y < 1\} < \infty,$$

where $\|\cdot\|_p$ stands for the standard norm in the space $L^p([a,b])$. Then $\mu_\varphi^{\mathrm{s}}((a,b)) = 0$.

(5) Let $(a,b) \cap \mathrm{spec}_{\mathrm{s}} A = \emptyset$. Then there is a dense subset $D \subset \mathscr{H}$ such that $\sup\{\|\mathrm{Im}\,\langle\varphi|R(\cdot+iy;A)\varphi\rangle\|_p : 0 < y < 1\} < \infty$ for every p, $1 < p \le +\infty$, and every $\varphi \in D$.

(6) $\mu_\varphi^{\mathrm{p}}((a,b)) = 0$ *if and only if*

$$\lim\limits_{y\to0+} y \int_a^b [\mathrm{Im}\,\langle\varphi|R(x+iy;A)\varphi\rangle]^2 \, dx = 0.$$

Lemma 2.8. *Let θ be a smooth strictly positive function on $[a,b]$ and $a, b \notin$* $\mathrm{spec_{pp}}\,A$. *Then*

$$\lim_{y \to +0} \frac{1}{\pi} \, \mathrm{Im} \int_a^b \langle \varphi | R(x+iy;A)\varphi \rangle \, dx$$

$$= \lim_{y \to +0} \frac{1}{\pi} \, \mathrm{Im} \int_a^b \langle \varphi | R(x+iy\theta(x);A)\varphi \rangle \, dx$$

$$= \lim_{y \to +0} \frac{y}{\pi} \int_a^b \| R(x+iy\theta(x);A)\varphi \|^2 \theta(x) \, dx. \quad (2.4)$$

Proof. The second equality in (2.4) follows from (2.1), so its is sufficient to prove the first equality only.

Rewrite the left-hand side of (2.4) as

$$\int_a^b \langle \varphi | R(x+iy;A)\varphi \rangle \, dx = \int_{\ell(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta, \quad (2.5)$$

where the path $\ell(y)$ is given in the coordinates $\zeta = \xi + i\eta$ by the equations: $\xi = t$, $\eta = y$, $t \in [a,b]$. Consider another path $\lambda(y)$ given by $\xi = t$, $\eta = y\theta(t)$, $t \in [a,b]$ and two vertical intervals: $v_1(y)$: $\xi = a$, η between y and $y\theta(a)$ and $v_2(y)$: $\xi = b$, η between y and $y\theta(b)$. Since the integrand in (2.5) is an analytic function, we can choose the orientation of the intervals $v_1(y)$ and $v_2(y)$ in such a way that

$$\int_{\ell(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta = \int_{\lambda(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta$$

$$+ \int_{v_1(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta + \int_{v_2(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta. \quad (2.6)$$

Suppose $\theta(a) \geq 1$ (the opposite case is considered similarly). Then

$$\int_{v_1(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta = \int_y^{y\theta(a)} \langle \varphi | R(a+i\eta;A)\varphi \rangle \, d\eta.$$

Let v_φ be the spectral measure associated with A and φ, then by Fubini

$$\mathrm{Im} \int_y^{y\theta(a)} \langle \varphi | R(a+i\eta;A)\varphi \rangle \, d\eta = \mathrm{Im} \int_y^{y\theta(a)} \int_{\mathbb{R}} \frac{dv_\varphi(t)}{t-a-i\eta} \, d\eta$$

$$= \int_y^{y\theta(a)} d\eta \, \eta \int_{\mathbb{R}} \frac{dv_\varphi(t)}{(t-a)^2+\eta^2} = \frac{1}{2} \int_{\mathbb{R}} \ln \frac{(t-a)^2+y^2\theta(a)^2}{(t-a)^2+y^2} \, dv_\varphi(t).$$

Using the estimate

$$\ln \frac{(t-a)^2+y^2\theta(a)^2}{(t-a)^2+y^2} = \ln \left(1 + \frac{y^2(\theta(a)^2-1)}{(t-a)^2+y^2} \right) \leq 2\ln \theta(a).$$

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and the boundedness of v_φ we obtain by the Lebesgue majorization theorem

$$\lim_{y\to 0+} \operatorname{Im} \int_{v_1(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta = 0. \tag{2.7a}$$

Exactly in the same way there holds

$$\lim_{y\to 0+} y \int_{v_2(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta = 0. \tag{2.7b}$$

On the other hand,

$$\operatorname{Im} \int_{\lambda(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta$$
$$= \operatorname{Im} \int_a^b \langle \varphi | R(x+iy\theta(x);A)\varphi \rangle \left(1+iy\theta'(x)\right) dx = I_1(y) + iyI_2(y), \tag{2.8}$$

where, by (2.1),

$$I_1(y) := \operatorname{Im} \int_a^b \langle \varphi | R(x+iy\theta(x);A)\varphi \rangle dx$$
$$\equiv y \int_a^b \left\| R(x+iy\theta(x);A)\varphi \right\|^2 dx,$$
$$I_2(y) := \operatorname{Im} \int_a^b \langle \varphi | R(x+iy\theta(x);A)\varphi \rangle \, \theta'(x) \, dx$$
$$\equiv y \int_a^b \left\| R(x+iy\theta(x);A)\varphi \right\|^2 \theta'(x) dx.$$

Denoting $c = \max_{x\in[a,b]} |\theta'(x)|$ one immediately obtains $|I_2(y)| \le c|I_1(y)|$. Therefore, passing to the limit $y \to 0+$ in (2.8) we arrive at

$$\lim_{y\to 0+} I_1(y) = \lim_{y\to 0+} \operatorname{Im} \int_{\lambda(y)} \langle \varphi | R(\zeta;A)\varphi \rangle \, d\zeta.$$

Substituting the latter equality, (2.7a), and (2.7b) in (2.6) results in (2.4). $\qquad\square$

3 Spectra and spectral measures for self-adjoint extensions

3.1 Problem setting and notation

In this section we return to self-adjoint extensions. Below

- S is a densely defined symmetric operator in $\mathscr{H}$ with equal deficiency indices in a Hilbert space $\mathscr{H}$,

- $\mathscr{N}_z := \ker(S^* - z)$,

- $(\mathscr{G}, \Gamma_1, \Gamma_2)$ is a boundary triple for S^*,

- Λ is a self-adjoint *operator* in $\mathscr{G}$,

- H^0 is the self-adjoint restriction of S^* to $\ker \Gamma_1$,

- H_Λ is the self-adjoint restriction of S^* to $\ker(\Gamma_2 - \Lambda\Gamma_1)$; due the the condition on Λ, H_Λ and H^0 are disjoint, see Remark 1.30.

- $R^0(z) := (H^0 - z)^{-1}$ for $z \in \operatorname{res} H^0$,

- $R_\Lambda(z) := (H_\Lambda - z)^{-1}$ for $z \in \operatorname{res} H_\Lambda$,

- γ is the Krein Γ-field induced by the boundary triple,

- Q is the Krein's $\mathscr{Q}$-function induced by the boundary triple.

Recall that the resolvent are connected by the Krein resolvent formula (theorem 1.29):

$$R_\Lambda(z) = R^0(z) - \gamma(z)\big[Q(z) - \Lambda\big]^{-1}\gamma^*(\bar{z}). \tag{3.1}$$

We are interested in the spectrum of H_Λ assuming that the spectrum of H^0 is known. Theorem 1.23 and Eq. (3.1) above show the equality

$$\operatorname{spec} H_\Lambda \setminus \operatorname{spec} H^0 = \Big\{ E \in \operatorname{res} H^0 : 0 \in \operatorname{spec}\big(Q(E) - \Lambda\big) \Big\}. \tag{3.2}$$

We are going to refine this correspondence in order to distinguish between different spectral types of H_Λ in gaps of H^0. Some of our results are close to that obtained in [24] for simple operators, but are expressed in different terms.

3.2 Discrete and essential spectra

The aim of the present subsection is to relate the discrete and essential spectra for H_Λ with those for $Q(z) - \Lambda$.

Lemma 3.1. *Let A and B be self-adjoint operators in $\mathscr{G}$, and A be bounded and strictly positive, i.e. $\langle \phi, A\phi \rangle \geq c\langle \phi, \phi \rangle$ for all $\phi \in \operatorname{dom} A$ with some $c > 0$. Then 0 is an isolated eigenvalue of B if and only if 0 is an isolated eigenvalue of ABA.*

Proof. Denote $L := ABA$. Let 0 is a non-isolated point of the spectrum of B. Then there is $\phi_n \in \operatorname{dom} B$ such that $B\phi_n \to 0$ and $\operatorname{dist}(\ker B, \phi_n) \geq \varepsilon > 0$. Set $\psi_n = A^{-1}\phi_n$. Then $L\psi_n \to 0$. Suppose that $\liminf \operatorname{dist}(\ker L, \psi_n) = 0$. Then there are $\psi'_n \in \ker L$ such that $\liminf \|\psi_n - \psi'_n\| = 0$. It is clear that $\phi'_n = A\psi'_n \in \ker B$ and $\liminf \|\phi_n - \phi'_n\| = \liminf \|A\psi_n - A\psi'_n\| = 0$. This contradiction shows that $\operatorname{dist}(\ker L, \psi_n) \geq \varepsilon' > 0$ and 0 is a non-isolated point of the spectrum of L.

The converse follows by symmetry, as A^{-1} is also positive definite. $\qquad\square$

Theorem 3.2. *For $E \in \operatorname{res} H^0$ the following assertions are equivalent:*

(1) E is an isolated point of the spectrum of H_Λ;

(2) 0 is an isolated point of the spectrum of $Q(E) - \Lambda$.

Moreover, if one of these conditions is satisfied, then for z in a punctured neighborhood of E there holds

$$\left\| \left(Q(z) - \Lambda \right)^{-1} \right\| \leq \frac{c}{|z - E|} \text{ for some } c > 0. \tag{3.3}$$

Proof. Clearly, one can assume that E is real. Denote $Q_0 := Q(E)$, $Q_1 := Q'(E)$. Both Q_0 and Q_1 are bounded self-adjoint operators. By (1.22a) there holds $Q_1 = \gamma^*(E)\gamma(E)$, therefore, Q_1 is positive definite. Take any $r < \operatorname{dist}(E, \operatorname{spec} H^0 \cup \operatorname{spec} H_\Lambda \setminus \{E\})$. For $|z - E| < r$ we have an expansion

$$Q(z) = Q_0 + (z - E)Q_1 + (z - E)^2 S(z), \tag{3.4}$$

where S is a holomorphic map from a neighborhood of E to $\mathbf{L}(\mathscr{G}, \mathscr{G})$.

$(1) \Rightarrow (2)$. Let E be an isolated point of the spectrum of H_Λ. Since E is an isolated point in the spectrum of H_Λ, the resolvent $R_\Lambda(z) \equiv (H_\Lambda - E)^{-1}$ has a first order pole at $z = E$, therefore, as follows from the resolvent formula (3.1), the function $z \mapsto \left(Q(z) - \Lambda \right)^{-1}$ also has a first order pole at the same point. Hence, we can suppose that for $0 < |z - E| < r$ there exists the bounded inverse $(Q(z) - \Lambda)^{-1}$ and, moreover, $\|(z - E)(Q(z) - \Lambda)^{-1}\| \leq c$ for some constant $c > 0$. This implies the estimate (3.3). By (3.4) we can choose r small enough, such that $Q_0 - \Lambda + (z - E)Q_1$ has a bounded inverse for $0 < |z - E| < r$. Representing

$$Q_0 - \Lambda + (z - E)Q_1 = Q_1^{1/2} \left(Q_1^{-1/2}(Q(E) - \Lambda)Q_1^{-1/2} + (z - E)I \right) Q_1^{1/2}$$

we see that 0 is an isolated point in the spectrum of $Q_1^{-1/2}(Q(E) - \Lambda)Q_1^{-1/2}$ and hence of $Q(E) - \Lambda$ in virtue of lemma 3.1.

$(2) \Rightarrow (1)$. Conversely, let 0 be an isolated point of the spectrum of $Q(E) - \Lambda$ or, which is equivalent by lemma 3.1, in the spectrum of $T := Q_1^{-1/2}(Q(E) -$

$\Lambda)Q_1^{-1/2}$. For sufficiently small r and $0 < |z - E| < r$ the operator $M(z) := T + (z - E)I$ is invertible, and $\|(z - E)M^{-1}(z)\| \le c'$ for these z for some constant c'. For the same z, the operator $Q_0 - \Lambda + (z - E)Q_1 \equiv Q_1^{1/2}M(z)Q_1^{1/2}$ is also boundedly invertible, and $\left\|(z - E)\left(Q_0 - \Lambda + (z - E)Q_1\right)^{-1}\right\| \le c''$. Hence, we can chose r such that $Q(z) - \Lambda = Q_0 - \Lambda + (z - E)Q_1 + (z - E)^2 S(z)$ is invertible for $0 < |z - E| < r$, which by (3.2) means that $z \notin \operatorname{res} H_\Lambda$. $\qquad\square$

Now we are able to refine the relationship (3.2) between the spectra of H^0 and H_Λ. This is the main result of the subsection.

Theorem 3.3. *The spectra of H and H_Λ are related by*

$$\operatorname{spec}_\bullet H_\Lambda \setminus \operatorname{spec} H^0 = \left\{ E \in \operatorname{res} H^0 : 0 \in \operatorname{spec}_\bullet \left(Q(E) - \Lambda\right)\right\} \qquad (3.5)$$

with $\bullet \in \{\mathrm{pp}, \mathrm{dis}, \mathrm{ess}\}$.

Proof. By theorem 1.23(1), Eq. (3.5) holds for $\bullet = \mathrm{pp}$, moreover, the multiplicities of the eigenvalues coincide in this case. Therefore, by theorem 3.2, the isolated eigenvalues of finite multiplicities for H_Λ correspond to the isolated zero eigenvalues for $Q(z) - E$, which proves (3.5) for $\bullet = \mathrm{dis}$. By duality this holds for the essential spectra too. $\qquad\square$

It is also useful to write down the spectral projector for H_Λ corresponding to isolated eigenvalues lying in $\operatorname{res} H^0$.

Proposition 3.4. *Let $E \in \operatorname{res} H^0$ be an isolated eigenvalue of H_Λ. Then the eigenprojector P_Λ for H_Λ corresponding to E is given by*

$$P_\Lambda = \gamma(E)\left(Q'(E)\right)^{-1/2}\Pi\left(Q'(E)\right)^{-1/2}\gamma^*(E),$$

where Π is the orthoprojector on $\ker\left(Q'(E)\right)^{-1/2}\left(Q(E) - \Lambda\right)\left(Q'(E)\right)^{-1/2}$ in $\mathscr{G}$.

Proof. Follows from the equality $P_\Lambda = -\operatorname{Res}\left[R_\Lambda(z); z = E\right]$. $\qquad\square$

3.3 Estimates for spectral measures

In this subsection we are going to obtain some information on the absolutely continuous, singular continuous, and point spectra of H_Λ using the asymptotic behavior of $\left(Q(x + iy) - \Lambda\right)^{-1}$ for $x \in \mathbb{R}$ and $y \to 0+$. To do this, we need first an expression for the resolvent R_Λ on the defect subspaces of S.

Lemma 3.5. *Let $\zeta, z \in \mathbb{C} \setminus \mathbb{R}$, $z \ne \zeta$, and $g \in \operatorname{dom}\Lambda$. For $\varphi = \gamma(\zeta)g$ there holds*
$$R_\Lambda(z)\varphi = \frac{1}{\zeta - z}\left[\varphi - \gamma(z)\left(Q(z) - \Lambda\right)^{-1}\left(Q(\zeta) - \Lambda\right)g\right].$$

Proof. Substituting identities (1.14b) and (1.21e) into (3.1) we obtain:

$$
\begin{aligned}
R_\Lambda(z)\varphi &= R^0(z)\gamma(\zeta)g - \gamma(z)\big[Q(z)-\Lambda\big]^{-1}\gamma^*(\bar{z})\gamma(\zeta)g \\
&= R^0(z)\gamma(\zeta)g - \gamma(z)\big[Q(z)-\Lambda\big]^{-1}\gamma^*(\bar{\zeta})\gamma(z)g \\
&= \frac{\gamma(z)-\gamma(\zeta)}{z-\zeta}g - \gamma(z)\big[Q(z)-\Lambda\big]^{-1}\frac{Q(z)-Q(\zeta)}{z-\zeta}g \\
&= \frac{1}{\zeta-z}\Big[\gamma(\zeta)g - \gamma(z)\big\{I - \big[Q(z)-\Lambda\big]^{-1} \\
&\quad\times \big(Q(z)-\Lambda+\Lambda-Q(\zeta)\big)\big\}g\Big] \\
&= \frac{1}{\zeta-z}\Big[\varphi - \gamma(z)\big(Q(z)-\Lambda\big)^{-1}\big(Q(\zeta)-\Lambda\big)g\Big].
\end{aligned}
$$

$\square$

Theorem 3.6. *Fix* $\zeta_0 \in \mathbb{C}\setminus\mathbb{R}$. *Let* $g \in \operatorname{dom}\Lambda$; *denote* $h := \big(Q(\zeta_0)-\Lambda\big)g$, $\varphi := \gamma(\zeta_0)g$, *and let* μ_φ *be the spectral measure for* H_Λ *associated with* φ.

(1) If $[a,b] \subset \operatorname{res}H^0 \cap \mathbb{R}$ *and* $a,b \notin \operatorname{spec}_{\mathrm{pp}}H_\Lambda$, *then*

$$
\begin{aligned}
\mu_\varphi([a,b]) &\equiv \big\|P_{[a,b]}(H_\Lambda)\varphi\big\|^2 \\
&= \lim_{y\to+0}\frac{y}{\pi}\int_a^b \frac{1}{|\zeta_0-x|^2}\big\|(Q'(x))^{1/2}\big(Q(x+iy)-\Lambda\big)^{-1}h\big\|^2\,dx.
\end{aligned}
$$

(2) For a.e. $x \in \operatorname{res}H^0 \cap \mathbb{R}$ *there exists the limit*

$$
f(x) := \lim_{y\to+0} y\big\|(Q'(x))^{1/2}\big(Q(x+iy)-\Lambda\big)^{-1}h\big\|^2,
$$

and the function $F(x) := \dfrac{1}{\pi|\zeta_0-x|^2}f(x)$ *is the Lebesgue density of the measure* $\mu_\varphi^{\mathrm{ac}}$, *i.e.* $\mu_\varphi^{\mathrm{ac}} = F(x)\,dx$.

(3) For $a \in \operatorname{res}H^0 \cap \mathbb{R}$ *the limit*

$$
\lim_{y\to+0} y^2\big\|(Q'(a))^{1/2}\big(Q(a+iy)-\Lambda\big)^{-1}h\big\|^2
$$

exists and is equal to $\mu_\varphi^{\mathrm{p}}(\{a\})$.

Proof. We start with proving item (2). Using lemma 3.5 we get for $y > 0$:

$$R_\Lambda(x+iy)\varphi = \frac{1}{\zeta_0 - x - iy}\,\varphi - \frac{1}{\zeta_0 - x - iy}\,\gamma(x+iy)\big[Q(x+iy)-\Lambda\big]^{-1}h,$$

therefore

$$\left|\,\left\|\sqrt{y}R_\Lambda(x+iy)\varphi\right\| - \left\|\frac{\sqrt{y}}{\zeta_0 - x - iy}\varphi\right\|\,\right|$$

$$\le \frac{\sqrt{y}}{|\zeta_0 - x - iy|}\left\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\|$$

$$\le \sqrt{y}\left\|R_\Lambda(x+iy)\varphi\right\| + \frac{\sqrt{y}}{|\zeta_0 - x - iy|}\left\|\varphi\right\|.$$

Hence, if $\sqrt{y}\|R_\Lambda(x+iy)\varphi\|$ has a limit (finite or infinite) as $y \to +0$, then also $\sqrt{y}\left\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\|$ does, and in this case

$$\lim_{y\to+0}\sqrt{y}\left\|R_\Lambda(x+iy)\varphi\right\|$$

$$= \frac{1}{|\zeta_0 - x|}\lim_{y\to+0}\sqrt{y}\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\|. \quad (3.6)$$

Let us show that, at fixed x, the finiteness of the limit (3.6) is equivalent to

$$\sup_{0<y<1}\sqrt{y}\left\|\big(Q(x+iy)-\Lambda\big)^{-1}h\right\| < \infty. \quad (3.7)$$

Indeed, since $\gamma(z)$ is a linear topological isomorphism on its image and is analytic, for a given $x \in \mathrm{res}\,H^0$ there exists $c > 0$ such that $c^{-1}\|g\| \le \sup_{0<y<1}\left\|\gamma(x+iy)g\right\| \le c\|g\|$ for all $g \in \mathscr{G}$. This shows that the conditions

$$\lim_{y\to+0}\sqrt{y}\left\|\gamma(x)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\| = +\infty$$

and

$$\lim_{y\to+0}\sqrt{y}\left\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\| = +\infty$$

are equivalent. Assume now $\lim_{y\to+0}\sqrt{y}\left\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\| < +\infty$, then for all $0 < y < 1$ one has

$$\left|\,\sqrt{y}\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h\| - \sqrt{y}\|\gamma(x)\big(Q(x+iy)-\Lambda\big)^{-1}h\|\,\right|$$

$$\le \sqrt{y}\left\|\gamma(x+iy)\big(Q(x+iy)-\Lambda\big)^{-1}h - \gamma(x)\big(Q(x+iy)-\Lambda\big)^{-1}h\right\|$$

$$\le c\left\|\gamma(x+iy)-\gamma(x)\right\|,$$

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where $c = \sup_{0 < y < 1} \sqrt{y} \left\| \left(Q(x+iy) - \Lambda \right)^{-1} h \right\| < \infty$. Thus, we have

$$\lim_{y \to +0} \sqrt{y} \left\| R_\Lambda(x+iy)\varphi \right\| = \frac{1}{|\zeta_0 - x|} \lim_{y \to +0} \sqrt{y} \left\| \gamma(x) \left(Q(x+iy) - \Lambda \right)^{-1} h \right\|. \quad (3.8)$$

On the other hand there holds

$$\left\| \gamma(x) \left(Q(x+iy) - \Lambda \right)^{-1} h \right\|^2$$
$$= \left\langle \gamma^*(x)\gamma(x) \left(Q(x+iy) - \Lambda \right)^{-1} h \,\middle|\, \left(Q(x+iy) - \Lambda \right)^{-1} h \right\rangle,$$

and, due to identities $\gamma^*(x)\gamma(x) \equiv Q'(x)$ and $\left\| \gamma(x) \left(Q(x+iy) - \Lambda \right)^{-1} h \right\|^2 = \left\| \left(Q'(x) \right)^{1/2} \left(Q(x+iy) - \Lambda \right)^{-1} h \right\|^2$, item (2) follows from proposition 2.7.

The proof of items (1) and (3) is completely similar to that for item (2); in the case of (1) one should use the norm

$$\|f\|_2 = \left(\int_a^b \|f(x)\|^2 \, dx \right)^{1/2}$$

on the space $L^2([a,b]; \mathcal{H})$ in the above estimates. $\qquad\square$

Below we will use the notation

$$\mathcal{H}_0 := \left(\bigcup_{\operatorname{Im}\zeta \neq 0} \ker(S^* - \zeta) \right)^\perp, \qquad \mathcal{H}_1 := \mathcal{H}_0^\perp.$$

For a subspace $L \subset \mathcal{G}$ we write $\mathcal{H}_1(L) := \bigcup_{\operatorname{Im}\zeta \neq 0} \gamma(\zeta) X_\zeta$ with $X_\zeta(L) = \left(Q(\zeta) - \Lambda \right)^{-1} L$. Note that if $\operatorname{span} L$ is dense in $\mathcal{G}$, then also $X_\zeta(L)$ is, and the linear hull of $\mathcal{H}_0 \cup \mathcal{H}_1(L)$ is dense in $\mathcal{H}$.

If $\psi \in \mathcal{H}_0$, then $\gamma^*(\zeta)\psi = 0$ for all $\zeta \in \mathbb{C} \setminus \mathbb{R}$. By (3.1), it follows $R_\Lambda(\zeta)\psi = R^0(\zeta)\psi$, and hence $\mu_\psi(\Omega) = 0$ for all Borel sets $\Omega \subset \operatorname{res} H^0 \cap \mathbb{R}$, where μ_ψ is the spectral measure for H_Λ associated with ψ.

Proposition 3.7 (cf. Theorem 2 from [62]). *Let $a, b \in \operatorname{res} H^0$. Suppose that there exists a subset $L \subset \mathcal{G}$ with dense $\operatorname{span} L$ such that*

$$\sup \left\{ \left\| \left(Q(x+iy) - \Lambda \right)^{-1} h \right\| : a < x < b, 0 < y < 1 \right\} < \infty$$

for all $h \in L$. Then $(a,b) \cap \operatorname{spec} H_\Lambda = \emptyset$.

Proof. We can assume that $a, b \notin \mathrm{spec}_{\mathrm{pp}} H_\Lambda$; otherwise we consider (a, b) as the union of a increasing sequence of intervals (a_n, b_n), where $a_n, b_n \notin \mathrm{spec}_{\mathrm{pp}} H_\Lambda$.

It is sufficient to show that $P_{(a,b)}(H_\Lambda) \mathscr{H}_1(L) = 0$. Let $\varphi \in \mathscr{H}_1(L)$, then there is $g \in L$ and $\zeta \in \mathbb{C} \setminus \mathbb{R}$ such that $\varphi = \gamma(\zeta)(Q(\zeta) - \Lambda)^{-1} g$. Using lemma 3.5 with $z = x + iy$ we get

$$R_\Lambda(x + iy)\varphi = \frac{1}{\zeta - x - iy}\left[\varphi - \gamma(x + iy)(Q(x + iy) - \Lambda)^{-1}g\right]. \qquad (3.9)$$

Using (2.3) we arrive at $P_{(a,b)}(H_\Lambda)\varphi = 0$. $\qquad\square$

Proposition 3.8. *For any $x_0 \in \mathrm{res}\, H^0 \cap \mathbb{R}$ the following two assertions are equivalent:*

(1) $x_0 \notin \mathrm{spec}\, H_\Lambda$;

(2) there exist $\varepsilon > 0$ and a subset $L \subset \mathscr{G}$ with dense $\mathrm{span}\, L$ such that $(x_0 - \varepsilon, x_0 + \varepsilon) \subset \mathrm{res}\, H^0$ and

$$\lim_{y \to +0} y \int_{x_0 - \varepsilon}^{x_0 + \varepsilon} \left\|(Q(x + iy) - \Lambda)^{-1}h\right\|^2 dx = 0.$$

for all $h \in L$.

Proof. The implication $(1) \Rightarrow (2)$ is trivial. Let us prove $(2) \Rightarrow (1)$.

It is sufficient to show that $\|P_{(x_0 - \varepsilon, x_0 + \varepsilon)}(H^\Lambda)\varphi\| = 0$ for all $\varphi \in \mathscr{H}_1(L)$. For a given $\varphi \in \gamma(\zeta)X_\zeta(L)$ with $\mathrm{Im}\, \zeta \neq 0$ we take $h \in L$ such that $h = (Q(\zeta) - \Lambda)g$, $\varphi = \gamma(\zeta)g$ for some $g \in \mathrm{dom}\,\Lambda$. Then the equality $\|P_{(x_0 - \varepsilon, x_0 + \varepsilon)}(H^\Lambda)\varphi\| = 0$ follows from theorem 3.6(1). $\qquad\square$

Proposition 3.9. *Let $a, b \in \mathrm{res}\, H^0$. Suppose that there exists a subset $L \subset \mathscr{G}$ with dense $\mathrm{span}\, L$ such that for all $h \in L$ and $x \in (a, b)$ there holds*

$$\sup\left\{\sqrt{y}\left\|(Q(x + iy) - \Lambda)^{-1}h\right\| : 0 < y < 1\right\} < \infty.$$

Then $(a, b) \cap \mathrm{spec}_s H_\Lambda = \emptyset$.

Proof. Let μ_φ be the spectral measure associated with φ and H_Λ. It is sufficent to show that $\mu_\varphi^s(a, b) = 0$ for all $\varphi \in \mathscr{H}_1(L)$. Writing any $\varphi \in \mathscr{H}_1(L)$ in the form $\varphi = \gamma(\zeta)(Q(\zeta) - \Lambda)^{-1} g$ with $g \in L$ and $\mathrm{Im}\, \zeta \neq 0$ one arrives again at (3.9). Therefore, for any $x \in (a, b)$ one has $\sup_{y \in (0,1)} \sqrt{y}\|R_\Lambda(x + iy)\varphi\| < \infty$, and $\mathrm{supp}\,\mu_\varphi^s \cap (a, b) = \emptyset$ by theorem 2.7(2). $\qquad\square$

Proposition 3.10. *Let $x_0 \in \operatorname{res} H^0 \cap \mathbb{R}$. Then the following assertions are equivalent:*

(1) $x_0 \notin \operatorname{spec}_{ac} H^\Lambda$;

(2) *there exist $\varepsilon > 0$ and a subset $L \subset \mathscr{G}$ with dense span L such that $(x_0 - \varepsilon, x_0 + \varepsilon) \subset \operatorname{res} H^0$ and $\lim_{y \to +0} \sqrt{y} (Q(x + iy) - \Lambda)^{-1} h = 0$ for all $h \in L$ and for a.e. $x \in (x_0 - \varepsilon, x_0 + \varepsilon)$.*

Proof. The proof of the implication $(2) \Rightarrow (1)$ is completely similar to that for proposition 3.8, cf. theorem 3.6(1)

To prove $(1) \Rightarrow (2)$ we take $\varepsilon > 0$ such that $(x_0 - \varepsilon, x_0 + \varepsilon) \cap \operatorname{spec}_{ac} H_\Lambda = \emptyset$. According to theorem 3.6(2) we have

$$\lim_{y \to +0} y \left\| \left(Q'(x)\right)^{1/2} \left(Q(x + iy) - \Lambda\right)^{-1} h \right\|^2 = 0$$

for all $h \in \mathscr{G}$, and it is sufficient to note that $\left(Q'(x)\right)^{1/2}$ is a linear topological isomorphism. $\qquad\square$

Proposition 3.11. *Let $x_0 \in \operatorname{res} H^0$. Then the following assertions are equivalent:*

(1) $x_0 \notin \operatorname{spec}_p H_\Lambda$;

(2) *there exist $\varepsilon > 0$ and a subset $L \subset \mathscr{G}$ with dense span L such that $(x_0 - \varepsilon, x_0 + \varepsilon) \subset \operatorname{res} H^0$ and $\lim_{y \to +0} y \left(Q(x + iy) - \Lambda\right)^{-1} h = 0$ for all $h \in L$ and for every $x \in (x_0 - \varepsilon, x_0 + \varepsilon)$.*

Proof. Similar to the proof of proposition 3.10 using theorem 3.6(3). $\qquad\square$

Using propositions 3.10 and 3.11 we get immediately

Proposition 3.12. *Let $x_0 \in \operatorname{res} H^0 \cap \operatorname{spec} H_\Lambda$. If for every $\varepsilon > 0$ there exists $h \in \mathscr{G}$ such that*

- $\lim_{y \to +0} y \left(Q(x + iy) - \Lambda\right)^{-1} h = 0$ *for all $x \in (x_0 - \varepsilon, x_0 + \varepsilon)$ and*

- $\lim_{y \to +0} \sqrt{y} \left(Q(x + iy) - \Lambda\right)^{-1} h = 0$ *for a.e. $x \in (x_0 - \varepsilon, x_0 + \varepsilon)$,*

then $x_0 \in \operatorname{spec}_{sc} H_\Lambda$.

3.4 Special $\mathscr{Q}$-functions

In this subsection we assume that the expression $Q(z) - \Lambda$ in the Krein forumula (3.1) has the following special form:

$$Q(z) - \Lambda = \frac{A - m(z)}{n(z)}, \tag{3.10}$$

where

- m and n are (scalar) analytic functions at least in $\mathbb{C} \setminus \mathbb{R}$,

- A is a self-adjoint operator in $\mathscr{G}$.

We assume that m and n admit analytic continuation to some interval $(a,b) \subset \operatorname{res} H^0 \cap \mathbb{R}$, moreover, they both are real and $n \neq 0$ in this interval.

Below, in subsections 3.5 and 3.6 we provide examples where such a situation arises. Our aim is to relate the spectral properties of H_Λ in (a,b) to the spectral properties of A. In what follows we denote by $\mathscr{J} := (\inf \operatorname{spec} A, \sup \operatorname{spec} A)$.

Lemma 3.13. *If n is constant, then m is monoton in (a,b). If n is non-constant and $m'(x) = 0$ for some $x \in (a,b)$, then either $m(x) < \inf \operatorname{spec} A$ or $m(x) > \sup \operatorname{spec} A$.*

Proof. For any $f \in \operatorname{dom} A$ consider the function $a_f(x) := \frac{1}{n(x)} \left\langle f \big| (A - m(x)) f \right\rangle$. Using (1.22a) we write

$$c\|f\|^2 \leq \left\langle f \big| Q'(x) f \right\rangle \equiv a'_f(x) = -\frac{m'(x)}{n(x)} \|f\|^2 - \frac{n'(x)}{n^2(x)} \left\langle f \big| (A - m(x)) f \right\rangle$$

with some constant $c > 0$ which is independent of f.

For constant n one has $n' \equiv 0$ and $-\dfrac{m'(x)}{n(x)} \geq c$, i.e. $m' \neq 0$.

If $n' \neq 0$ and $m'(x) = 0$, then $\dfrac{n'(x)}{n^2(x)} \left\langle f \big| (A - m(x)) f \right\rangle \geq c\|f\|^2$ for any f, i.e. the operator $A - m(x)$ is either positive definite or negative definite. $\qquad \square$

Lemma 3.14. *Let K be a compact subset of $(a,b) \cap m^{-1}(\overline{\mathscr{J}})$, then there is $y_0 > 0$ such that for $x \in K$ and $0 < y < y_0$ one has*

$$\left(Q(x+iy) - \Lambda \right)^{-1} = n(x+iy) L(x,y) \left[A - m(x) - iy m'(x) \right]^{-1}, \tag{3.11}$$

where $L(x,y)$ is a bounded operator and $\|L(x,y) - I\| \to 0$ uniformly with respect to $x \in K$ as $y \to 0$.

Proof. We have $\left(Q(x+iy) - \Lambda \right)^{-1} = n(x+iy)\left(A - m(x+iy) \right)^{-1}$. Further, $A - m(x+iy) = A - m(x) - iym'(x) + B(x,y)$, where $\|B(x,y)\| = O(y^2)$ uniformly with respect to $x \in K$. Since $m'(x) \neq 0$ for $x \in K$ by lemma 3.13, the operator $A - m(x) - iym'(x)$ has a bounded inverse defined everywhere, and

$$A - m(x+iy) = \left(A - m(x) - iym'(x) \right)\left[1 + \left(A - m(x) - iym'(x) \right)^{-1} B(x,y) \right].$$

It is easy to see that $\left\| \left(A - m(x) - iym'(x) \right)^{-1} \right\| = O\left(|y|^{-1} \right)$ uniformly with respect to $x \in K$. Therefore, for sufficiently small y,

$$\left(A - m(x+iy) \right)^{-1} = \left(1 + B_1(x,y) \right)^{-1}\left[A - m(x) - iym'(x) \right]^{-1}$$

with $\|B_1(x,y)\| = O\left(|y| \right)$ uniformly with respect to $x \in K$. $\qquad\square$

Lemma 3.15. *Fix ζ_0 with $\operatorname{Im}\zeta_0 \neq 0$ and let $h \in \mathscr{G}$, $\varphi = \gamma(\zeta_0)\left(Q(\zeta_0) - \Lambda \right)^{-1} h$. Denote by μ the spectral measure for the pair (H_Λ, φ) and by ν the spectral measure for the pair (A, h). There is a constant $c > 0$ with the following property: for any segment $K := [\alpha, \beta] \subset (a,b) \cap m^{-1}(\overline{\mathscr{J}})$ such that $\alpha, \beta \notin \operatorname{spec}_{\mathrm{pp}} H_\Lambda$ there holds $\mu(K) \leq c\nu\left(m(K) \right)$.*

Proof. Note first that $m' \neq 0$ on $[\alpha, \beta]$. To be definite, we suppose $m' > 0$. According to theorem 3.6(1) and lemma 3.14, we have

$$\mu(K) = \lim_{y \to +0} \frac{y}{\pi} \int_K \frac{n^2(x)}{|\zeta_0 - x|^2} \left\| \left(Q'(x) \right)^{1/2}\left(A - m(x) - iym'(x) \right)^{-1} h \right\|^2 dx.$$

Substituting $\xi := m(x)$ and denoting $\tau(\xi) := m'\left(m^{-1}(\xi) \right)$ we arrive at

$$\mu(K) = \lim_{y \to +0} \frac{y}{\pi} \int_{m(K)} \frac{n\left(m^{-1}(\xi) \right)^2}{\tau(\xi) \cdot |\zeta_0 - m^{-1}(\xi)|^2}$$
$$\times \left\| \left(Q'\left(\vartheta^{-1}(\xi) \right) \right)^{1/2}\left(A - \xi - iy\tau(\xi) \right)^{-1} h \right\|^2 d\xi.$$

Since

$$\int_{m(K)} \frac{n\left(m^{-1}(\xi) \right)^2}{\tau(\xi) \cdot |\zeta_0 - m^{-1}(\xi)|^2} \left\| \left(Q'\left(\vartheta^{-1}(\xi) \right) \right)^{1/2}\left(A - \xi - iy\tau(\xi) \right)^{-1} h \right\|^2 d\xi,$$
$$\leq c \int_{m(K)} \left\| \left(A - \xi - iy\tau(\xi) \right)^{-1} h \right\|^2 d\xi,$$

where c is independent of K, we obtain the result with the help lemma 2.8. $\qquad\square$

Here is the main result of the subsection.

Theorem 3.16. *Assume that the term $Q(z) - \Lambda$ in the Krein resolvent formula* (3.1) *admits the representation* (3.10), *then for any $x_0 \in \operatorname{spec} H_\Lambda \cap (a,b)$ and any $\bullet \in \{\mathrm{dis}, \mathrm{ess}, \mathrm{pp}, \mathrm{p}, \mathrm{ac}, \mathrm{s}, \mathrm{sc}, \mathrm{c}\}$ the conditions*

($\bullet$) $x_0 \in \operatorname{spec}_\bullet H_\Lambda$,

(m–$\bullet$) $m(x_0) \in \operatorname{spec}_\bullet A$

are equivalent.

Proof. For $\bullet = \mathrm{pp}, \mathrm{dis}, \mathrm{ess}$ see theorem 3.3. As m is a homeomorphism, the same holds for $\operatorname{spec}_\mathrm{p} \equiv \operatorname{spec}_\mathrm{pp}$.

For $\bullet = \mathrm{ac}$ use the following sequence of mutually equivalent assertions:

- $m(x_0) \notin \operatorname{spec}_\mathrm{ac} A$,

- There is a neighborhood V of $m(x_0)$ such that $y\|(A - \xi - iy)^{-1})h\|^2 \xrightarrow{y \to 0+} 0$ for all $\xi \in V$ and $h \in \mathscr{G}$ (use item 1 of theorem 2.7),

- There is a neighborhood W of x_0 such that $y\|(Q(x+iy) - \Lambda)^{-1})h\|^2 \xrightarrow{y \to 0+} 0$ for all $\xi \in W$ and $h \in \mathscr{G}$ (use lemma 3.14 and replace $iym'(x)$ at any fixed x by iy),

- $x_0 \notin \operatorname{spec}_\mathrm{ac} H_\Lambda$ (proposition 3.10).

Assume now $m(x_0) \in \operatorname{spec}_\mathrm{sc} A$. There exists a neighborhood V of $m(x_0)$ such that for some $h \in \mathscr{G}$ we have $v_h^\mathrm{ac}(V) = v_h^\mathrm{p}(V) = 0$, where v stands for the spectral measure for A. Using lemma 3.14 and theorem 2.7 one can see that there exists a neighborhood W of x_0 such that $\lim_{y \to +0} y^2\|(Q(x+iy) - \Lambda)^{-1}h\|^2 = 0$ for all $x \in W$ and $\lim_{y \to +0} y\|(Q(x+iy) - \Lambda)^{-1}h\|^2 = 0$ for a.e. $x \in W$. By proposition 3.12 this means that $x_0 \in \operatorname{spec}_\mathrm{sc}(H_\Lambda)$. Hence, we prove (m-sc)$\Rightarrow$(sc). Since $\operatorname{spec}_\mathrm{s} A = \operatorname{spec}_\mathrm{p} A \cup \operatorname{spec}_\mathrm{sc} A$, we prove also that (m-s)$\Rightarrow$(s).

Let now $m(x_0) \notin \operatorname{spec}_\mathrm{s} A$. To show that $x_0 \notin \operatorname{spec}_\mathrm{s} H_\Lambda$ it is sufficient to consider the case $m(x_0) \in \operatorname{spec} A \setminus \operatorname{spec}_\mathrm{s} A$. Then by theorem XIII.20 from [117], there exist a dense subset $L \subset \mathscr{G}$ and a neighborhood V of $m(x_0)$ such that

$$\sup \left\{ \|(A - \xi - iy)^{-1}h\| : 0 < y < 1, \ \xi \in V \right\} < \infty$$

for all $h \in L$. We can assume without loss of generality that $m'(x_0) > 0$, then by lemma 3.14 we have for a neighborhood W of x_0 and for some y_0, $y_0 > 0$,

$$\sup \left\{ \sqrt{y}\|(Q(x+iy) - \Lambda)^{-1}h\| : \ 0 < y < y_0, \ x \in W \right\} < \infty,$$

and $x_0 \notin \mathrm{spec_s}\, H_\Lambda$ by proposition 3.9. Thus, the equivalence (s)⇔(m-s) is proven.

Now we prove the impication (sc)⇒(m-sc). Assume that $x_0 \in \mathrm{spec_{sc}}(H_\Lambda)$ but $m(x_0) \notin \mathrm{spec_{sc}}\, A$. Denote the spectral measure for A by ν and that for H_Λ by μ, then there is an interval I containing x_0 such that for $J = m(I)$ there holds: $\nu_h^{\mathrm{sc}}(J) = 0$ for all $h \in \mathcal{G}$. According to lemma 3.15, if X is a Borel subset of I such that $\nu_h\big(m(X)\big) = 0$ for all h, then also $\mu_\varphi(X) = 0$ for all $\varphi \in \mathcal{H}_1$. In particular, let X be a Borel subset of I of zero Lebesgue measure and containing no eigenvalues of H_Λ. Then $m(X)$ is a Borel subset of J which contains no eigenvalues of A and also has the Lebesgue measure zero. Therefore $\nu_h\big(m(X)\big) = 0$, and hence $\mu_\varphi(X) = 0$. We see, that the restriction of μ_φ to I is mutually singular with each singular continuous measure on I. Hence, it is true for μ_φ with each $\varphi \in \mathcal{H}$. This contradicts to the assumption $x_0 \in \mathrm{spec_{sc}}\, H_\Lambda$, and the implication (sc)⇒(m-sc) is proven.

The equivalence (c)⇔(m-c) follows from (sc)⇔(m-sc) and (ac)⇔(m-ac). □

We note that theorem 3.16 may be considered as an abstract version of the dimension reduction: we reduce the spectrum problem for self-adjoint extensions to a spectral problem "on the boundary", i.e. in the space $\mathcal{G}$.

3.5 Spectral duality for quantum and combinatorial graphs

We have already mentioned that the theory of self-adjoint extensions has obvious applications in the theory of quantum graphs. Here we are going to develop the results of the recent paper [109] concerning the relationship between the spectra of quantum graphs and discrete Laplacians using theorem 3.16. Actually, this problem was the starting point of the work.

Let G be a countable directed graph. The sets of the vertices and of the edges of G will be denoted by V and E, respectively. We do not exclude multiple edges and self-loops. For an edge $e \in E$ we denote by ιe its initial vertex and by τe its terminal vertex. For a vertex v, the number of outgoing edges (outdegree) will be denoted by $\mathrm{outdeg}\, v$ and the number of ingoing edges (indegree) will be denoted by $\mathrm{indeg}\, v$. The degree of v is $\deg v := \mathrm{indeg}\, v + \mathrm{outdeg}\, v$. In what follows we assume that the degrees of the vertices of G are uniformly bounded, $1 \le \deg v \le N$ for all $v \in V$, in particular, there are no isolated vertices. Note that each self-loop at v counts in both $\mathrm{indeg}\, v$ and $\mathrm{outdeg}\, v$.

By identifying each edge e of G with a copy of the segment $[0,1]$, such that 0 is identified with the vertex ιe and 1 is identified with the vertex τe, one obtain a certain topological space. A magnetic Schrödinger operator in such a structure is defined as follows. The state space of the graph is $\mathcal{H} = \bigoplus_{e \in E} \mathcal{H}_e$, $\mathcal{H}_e = L^2[0,1]$, consisting of functions $f = (f_e)$, $f_e \in \mathcal{H}_e$. On each edge consider the same scalar potential $U \in L^2[0,1]$. Let $a_e \in C^1[0,1]$ be real-valued magnetic potentials on

the edges $e \in E$. Associate with each edge a differential expression $L_e := (i\partial + a_e)^2 + U$. The maximal operator which can be associated with these differential expressions acts as $(g_e) \mapsto (L_e g_e)$ on functions $g \in \bigoplus H^2[0,1]$. The integration by parts shows that this operator is not symmetric, and it is necessary to introduce boundary conditions at the vertices to obtain a self-adjoint operator. The standard self-adjoint boundary conditions for magnetic operators are

$$g_e(1) = g_b(0) =: g(v) \quad \text{for all } b,e \in E \text{ with } \iota b = \tau e = v,$$
$$\sum_{e:\iota e=v} \left(g_e'(0) - ia_e(0)g_e(0)\right) - \sum_{e:\tau e=v} \left(g_e'(1) - ia_e(1)g_e(1)\right) = \alpha(v)g(v),$$

where $\alpha(v)$ are real numbers, the so-called coupling constants. The gauge transformation $g_e(t) = \exp\left(i \int_0^t a_e(s)ds\right) f_e(t)$ removes the magnetic potentials from the differential expressions, $\left((i\partial + a_e)^2 + U\right)g_e = -f_e'' + Uf_e$, but the magnetic field enters the boundary conditions through the parameters $\beta(e) = \int_0^1 a_e(s)\,ds$ in the following way:

$$e^{i\beta(e)} f_e(1) = f_b(0) =: f(v) \quad \text{for all } b,e \in E \text{ with } \iota b = \tau e = v, \tag{3.12a}$$
$$f'(v) := \sum_{e:\iota e=v} f_e'(0) - \sum_{e:\tau e=v} e^{i\beta(e)} f_e'(1) = \alpha(v)f(v). \tag{3.12b}$$

The self-adjoint operator in $\mathscr{H}$ acting as $(f_e) \mapsto (-f_e'' + Uf_e)$ on functions $(f_e) \in \bigoplus H^2[0,1]$ satisfying the boundary conditions (3.12a) and (3.12b) for all $v \in V$ will be denoted by H. This is our central object.

To describe the spectrum of H let us make some preliminary constructions. We introduce a discrete Hilbert space $l^2(G)$ consisting of functions on V which are summable with respect to the weighted scalar product $\langle f,g \rangle = \sum_{v \in V} \deg v \, \overline{f(v)}g(v)$. Consider an arbitrary function $\beta : E \to \mathbb{R}$ and consider the corresponding discrete magnetic Laplacian in $l^2(G)$,

$$\Delta_G h(v) = \frac{1}{\deg v}\left(\sum_{e:\iota e=v} e^{-i\beta(e)} h(\tau e) + \sum_{e:\tau e=v} e^{i\beta(e)} h(\iota e)\right). \tag{3.13}$$

This expression defines a bounded self-adjoint operator in $l^2(G)$.

Denote by D the Dirichlet realtizetion of $-d^2/dt^2 + U$ on the segment $[0,1]$, $Df = -f'' + Uf$, $\operatorname{dom} D = \{f \in H^2[0,1] : f(0) = f(1) = 0\}$. The spectrum of D is a discrete set of simple eigenvalues.

For any $z \in \mathbb{C}$ denote by $s(\cdot;z)$ and $c(x;z)$ the solutions to $-y'' + Uy = zy$ satisfying $s(0;z) = c'(0;z) = 0$ and $s'(0;z) = c(0;z) = 1$. Introduce an extension of H, Π, defined by $\operatorname{dom} \Pi = \{f \in \bigoplus H^2[0,1] : \text{Eq. (3.12a) holds}\}$ and $\Pi(f_e) = (-f_e'' + Uf_e)$. The following proposition is proved in [109].

Proposition 3.17. *The operator Π is closed. For $f \in \operatorname{dom}\Pi$ put*

$$\Gamma_1 f = \big(f(v)\big)_{v \in V}, \quad \Gamma_2 f = \left(\frac{f'(v)}{\deg v}\right)_{v \in V}$$

with $f(v)$ and $f'(v)$ given by (3.12), then $\big(l^2(G), \Gamma_1, \Gamma_2\big)$ is a boundary triple for Π. The induced Γ-field γ and $\mathcal{Q}$-function Q are of the form

$$\big(\gamma(z)h\big)_e(x) = \frac{1}{s(1;z)}\Big[h(\iota e)\big(s(1;z)c(x;z) - s(x;z)c(1;z)\big) + e^{-i\beta(e)}h(\tau e)s(x;z)\Big],$$

and

$$Q(z)f(v) = \frac{1}{\deg v\, s(1;z)}\Big(\Delta_G - \big[\operatorname{outdeg} v\, c(1;z) + \operatorname{indeg} v\, s'(1;z)\big]\Big)f(v).$$

Now let us make some additional assumptions. We will say that the *symmetry condition* is satisfied if *at least one* of the following properties holds: $\operatorname{indeg} v = \operatorname{outdeg} v$ for all $v \in V$ *or U is even*, i.e. $U(x) = U(1-x)$.

The following theorem provides a complete description of the spectrum of the quantum graph H outside $\operatorname{spec} D$ in terms of the discrete Laplacian Δ_G.

Theorem 3.18. *Let the symmetry condition be satisfied and the coupling constants $\alpha(v)$ be of the form $\alpha(v) = \dfrac{\deg v}{2}\alpha$, then $\operatorname{spec}_{\bullet} \Lambda \setminus \operatorname{spec} D = \eta^{-1}(\operatorname{spec}_{\bullet}\Delta_G) \setminus \operatorname{spec} D$ for $\bullet \in \{\mathrm{dis}, \mathrm{ess}, \mathrm{pp}, \mathrm{p}, \mathrm{ac}, \mathrm{s}, \mathrm{sc}, \mathrm{c}\}$, where $\eta(z) = \dfrac{1}{2}\Big(s'(1;z) + c(1;z) + \alpha s(1;z)\Big)$.*

Proof. Let the symmetry conditions be satisfied. If U is even, then $s'(1;z) \equiv c(1;z)$. If $\operatorname{outdeg} v = \operatorname{indeg} v$ for all v, then $\operatorname{outdeg} v = \operatorname{indeg} v = \dfrac{1}{2}\deg v$. In both cases one has $Q(z) = \dfrac{2\Delta_G - s'(1;z) - c(1;z)}{2s(1;z)}$ (see [109] for a more detailed discussion). The operator H itself is the restriction of Π to the functions f satisfying $\Gamma_2 = \dfrac{\alpha}{2}\Gamma_1 f$ with $\Gamma_{1,2}$ from proposition 3.17. The restriction H^0 of S to $\ker\Gamma_1$ is nothing but the direct sum of the operators D over all edges. By theorem 1.29, the resolvents of H and H_0 are related by the Krein resolvent formula and, in particular, the corresponding term $Q(z) - \Lambda$ has the form $Q(z) - \Lambda = \dfrac{\Delta_G - \eta(z)}{s(1;z)}$, and we are in the situation of theorem 3.16. $\qquad\square$

3.6 Array-type systems

Another situation in which theorem 3.16 becomes useful appears when the $\mathscr{Q}$-function is of scalar type [5], i.e. when $Q(z)$ is just the multiplication by a certain complex function; such functions are of interest in the invesre spectral problem for self-adjoint extensions [23]. In this case the representition (3.10) holds for any self-adjoint operator Λ, and one has

Proposition 3.19. *Let Q be of scalar type, then for any Λ there holds* $\operatorname{spec}_\bullet H_\Lambda \setminus \operatorname{spec} H^0 = Q^{-1}(\operatorname{spec}_\bullet \Lambda) \setminus \operatorname{spec} H^0$ *with* $\bullet \in \{\mathrm{dis}, \mathrm{ess}, \mathrm{pp}, \mathrm{p}, \mathrm{ac}, \mathrm{s}, \mathrm{sc}, \mathrm{c}\}$.

In other words, the nature of the spectrum of the "perturbed" operator H_Λ in the gaps of the "unperturbed" operator H^0 is completely determined in terms of the parameter Λ.

Scalar type $\mathscr{Q}$-functions arise, for example, as follows. Let $\mathscr{H}_0$ be a separable Hilbert space and S_0 be a closed symmetric operator in $\mathscr{H}_0$ with the deficiency indices $(1,1)$. Let $(\mathbb{C}, \Gamma_1^0, \Gamma_2^0)$ be a boundary triple for the adjoint S_0^*, and $\gamma_0(z)$ and $q(z)$ be the induced Γ-field and $\mathscr{Q}$-function. Let D be the restriction of S_0^* to $\ker \Gamma_1^0$; this is a self-adjoint operator.

Let $\mathscr{A}$ be a certain countable set. Consider the operator $S := \bigoplus_{\alpha \in \mathscr{A}} S_\alpha$ in the space $\mathscr{H} := \bigoplus_{\alpha \in \mathscr{A}} \mathscr{H}_e$, where $\mathscr{H}_\alpha \simeq \mathscr{H}_0$ and $S_\alpha = S_0$. Clearly, $(l^2(\mathscr{A}), \Gamma_1, \Gamma_2)$ with $\Gamma_1(f_\alpha) = (\Gamma_1^0 f_\alpha)$ and $\Gamma_2(f_\alpha) = (\Gamma_2^0 f_\alpha)$ becomes a boundary triple for S^*. The induced Γ-field is $\gamma(z)(\xi_\alpha) = (\gamma_0(z)\xi_\alpha)$ and the $\mathscr{Q}$-function is scalar, $Q(z) = q(z)\mathrm{id}$. It is worthy to note that the corresponding operator H^0, which is the restriction of S^* to $\ker \Gamma_1$, is just the direct sum of the copies of D over the set $\mathscr{A}$ and, in particular, $\operatorname{spec} H^0 = \operatorname{spec} D$. Proposition 3.19 becomes especially useful if the spectrum of D is a discrete set, then the spectrum of H_Λ is (almost) completely determined in terms of the parameterizing operator Λ.

The models of the above type can be used for the construction of solvable models for array of quantum dots and antidots. One of pecularities of such arrays is that they involve the miscroscopic properties of a single point as well as the macropscopic properties of the whole system. We consider for technical simplicity two-dimensional periodic arrays in a uniform magnetic field orthogonal to the plane of the system. For a large class of such models we refer to [64].

Let $\mathbf{a}_1$, $\mathbf{a}_2$ be linearly independent vectors of $\mathbb{R}^2$ and $\mathscr{A}$ be the lattice spanned by them, $\mathscr{A} := \mathbb{Z}\mathbf{a}_1 + \mathbb{Z}\mathbf{a}_2$. Assume that each note α of the lattice is occupied by a certain object (quantum dot) whose state space is $\mathscr{H}_\alpha$ with a Hamiltonian H_α (their concrete form will be given later). We assume that all quantum dots are identical, i.e. $\mathscr{H}_\alpha := \mathscr{H}_0$, $H_\alpha = H_0$. The system is subjected to a uniform field orthogonal to the plane.

In our case, the inner state space $\mathscr{H}_0$ will be $L^2(\mathbb{R}^2)$. The Hamiltonian H_0 will

be taken in the form

$$H_0 = -\frac{1}{2}\left[\left(\frac{\partial}{\partial x} + \pi i\xi y\right)^2 + \left(\frac{\partial}{\partial y} - \pi i\xi x\right)^2\right] + \frac{\omega^2}{2}(x^2 + y^2).$$

Here ξ is the number of magnetic flux quanta thorugh a unit area segment of the plane, and ω is the strength of the quantum dot potential. Note that the spectrum of H^0 is pure point and consists of the infinite degenerate eigenvalues E_{mn},

$$E_{mn} = \frac{1}{2}(n+m+1)\Omega + (n-m)\xi, \quad \Omega := 2\sqrt{\pi^2\xi^2 + \omega^2}, \quad m,n \in \mathbb{Z}, \quad m,n \geq 0.$$

The Hamiltonian $H := \oplus_{\alpha \in \mathscr{A}} H_\alpha$, describe the array of non-interacting quantum dots. To take into account the interdot interaction we use the restriction-extnesion procedure. Namely denote by S_α the restriction of H_α to the functions vanishing at the origin. As we have shown in subsubsection 1.4.3, these operators are closed and have deficiency indices $(1,1)$. Respectively, one can construct the corrsponding boundary triples for S_α^*. Namely, for $f_\alpha \in \mathrm{dom}\, S_\alpha^*$ we denote

$$a(f_\alpha) := -\lim_{r \to 0} \frac{\pi}{\log|r|} f_\alpha(r), \quad b(f_\alpha) := \lim_{r \to 0}\left[f(r) + a(f_\alpha)\frac{1}{\pi}\log|r|\right].$$

Accoriding to the constructions of subsubsection 1.4.3, $(\mathbb{C}, a, b)$ form a boundary triple for S_α^*, and the corresponding $\mathscr{Q}$-function is

$$q(z) = -\frac{1}{2\pi}\left[\psi\left(\frac{1}{2} - \frac{z}{\Omega}\right) + \log\frac{\Omega}{2\pi} + 2C_E\right],$$

where ψ is the logarithmic derivative of the Γ function and C_E is the Euler constant.

Respectively, the triple $(l^2(\mathscr{A}), \Gamma_1, \Gamma_2)$ with

$$\Gamma_1(f_\alpha) := (a(f_\alpha)), \quad \Gamma_2(f_\alpha) := (b(f_\alpha)),$$

is a boundary triple for the operator S^*, $S := \oplus S_\alpha$, and the induced $\mathscr{Q}$-function is the multiplication by $q(z)$.

The above defined operator H corresponds exactly to the boundary condition $\Gamma_1 f = 0$. For a self-adjoint operator L in $l^2(\mathscr{A})$ denote by H_L the self-adjoint extension of S corresponding to the boundary conditions $\Gamma_2 f = L\Gamma_1 f$. This operator will be considered as a Hamiltonian of interacting quantum dots, and the way how different nodes interact with each other is determined by the operator L. To avoid technical difficulties we assume that L is bounded. Furthermore, L must satisfy some additional assumptions in order to take into account the nature of the problem.

First, any reasonable definition of a periodic system with magnetic field must include the invariance under the magnetic translation group. In our case this means that the matrix of L in the standard basis of $l^2(\mathscr{A})$ satisfies

$$L(\alpha, \alpha + \beta) = e^{\pi i \xi \alpha \wedge \beta} L(0, \beta) \quad \text{for any} \quad \alpha, \beta \in \mathscr{A}.$$

Second, we assume that only the nearest neighbors interact with each other, i.e.

$$L(\alpha, 0) = \begin{cases} \lambda_1, & \alpha = \pm \mathbf{a}_1, \\ \lambda_2, & \alpha = \pm \mathbf{a}_2, \\ 0, & \text{otherwise}, \end{cases} \quad \lambda_1, \lambda_2 \in \mathbb{R} \setminus \{0\}.$$

Roughly speaking, the above assumptions mean the following: each node interact α with the four nearest nodes $\alpha \pm \mathbf{a}_j$, $j = 1, 2$, and the interaction is independent of α. For further analysis it is useful to idenitfy $l^2(\mathscr{A})$ with $l^2(\mathbb{Z}^2)$ by $(f_{n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2}) \sim (f(n_1, n_2))$, $n_1, n_2 \in \mathbb{Z}$. Then the operator L acts as follows:

$$Lf(n_1, n_2) \equiv L(\eta) f(n_1, n_2) = \lambda_1 \left[e^{i\pi\eta n_2} f(n_1 - 1, n_2) + e^{-i\pi\eta n_2} f(n_1 + 1, n_2) \right]$$
$$+ \lambda_2 \left[e^{-i\pi\eta n_1} f(n_1, n_2 - 1) + e^{i\pi\eta n_1} f(n_1, n_2 + 1) \right], \quad \eta = \xi \mathbf{a}_1 \wedge \mathbf{a}_2.$$

This operator $L(\eta)$ is well-known and is called the *discrete magnetic Laplacian*, and using proposition 3.19 we can transfer the complete spectral information for L to the Hamiltonian of quantum dots H_L. One of interesting moments in the spectral analysis of L is the relationship with the almost Mathieu operator in the space $l^2(\mathbb{Z})$ [120],

$$M(\eta, \theta) f(n) = \lambda_1 \left[f(n-1) + f(n+1) \right] + 2\lambda_2 \cos\left(2\pi\eta n + \theta\right) f(n), \quad \theta \in [-\pi, \pi).$$

In particular,

$$\operatorname{spec} L(\eta) = \overline{\bigcup_{\theta \in [-\pi, \pi)} \operatorname{spec} M(\eta, \theta)}.$$

Elementary constructions of the Bloch analysis show that the spectrum of $L(\eta)$ is absolutely continuous and has a band structure. At the same time, for irrational η the spectrum of $M(\eta, \theta)$ is independent of θ and hence coincides with the spectrum of $L(\eta)$. It was shown only recently that the spectrum of $M(\eta, \theta)$ is a Cantor set for all irrational η and non-zero λ_1, λ_2, see [14]. Using our analysis we can claim that, up to the discrete set $\{E_{m,n}\}$ (a more precise analysis shows that these eigenvalues are all in the spectrum of the array) we can transfer the spectral information for $L(\eta)$ to the array of quantum dots; in particular, we obtain a Cantor spectrum for irrational η due to the analyticity of the $\mathscr{Q}$-function.

4 Isolated eigenvalues

4.1 Problem setting

In the previous sections we have analyzed the part of the spectrum of the "perturbed" operator H_Λ lying in the resolvent set of the "unperturbed" operator H^0. If $E \in \operatorname{spec} H^0$, then, in general, it is difficult to determine whether or not $E \in \operatorname{spec} H_\Lambda$. Nevertheless, if E is an isolated eigenvalue of H^0, then the question whether E in the spectrum of H_Λ becomes easier in comparison with the general case. (Examples of subsections 3.5 and 3.6 show that this situation is rather typical for applications.) In this section we give a necessary and sufficient condition for such an E to be an isolated eigenvalue of H_Λ and completely describe the corresponding eigensubspace of H_Λ (theorem 4.7). For simplicity, we consider only the case of *bounded* self-adjoint operator Λ in $\mathscr{G}$.

In addition to the notation given in subsection 3.1, in this section ε^0 denotes an eigenvalue of H^0 with the eigensubspace $\mathscr{H}^0$ (which can be infinite-dimensional), P^0 denotes the orthoprojector on $\mathscr{H}^0$. We denote by $\mathscr{V}(\varepsilon^0)$ the set of all open balls $\mathscr{O}$ centered at ε^0 and such that $\operatorname{spec} H^0 \cap \mathscr{O} = \{\varepsilon^0\}$. By $\mathbf{GL}(\mathscr{G})$ we denote the set of bounded linear operators in $\mathscr{G}$ having a bounded inverse. If $\mathscr{O} \in \mathscr{V}(\varepsilon^0)$, then $\mathbf{K}(\mathscr{O};\mathscr{G})$ denotes the space of all analytic mappings $V : \mathscr{O} \to \mathbf{GL}(\mathscr{G})$ such that $V(\varepsilon^0) = I$ and $V^*(\bar{z}) = V^{-1}(z)$ (the latter condition is equivalent to the following one: $V(z)$ is a unitary operator for $z \in \mathbb{R} \cap \mathscr{O}$).

4.2 Auxiliary constructions

Further we need the following lemma.

Lemma 4.1. *For any $z, \zeta \in \operatorname{res} H^0$ there holds:*

(1) $P^0 \mathscr{N}_z = P^0 \mathscr{N}_\zeta$;

(2) $\mathscr{H}^0 \cap \operatorname{dom} H_\Lambda = \mathscr{H}^0 \cap \mathscr{N}_z^\perp = \mathscr{H}^0 \ominus \operatorname{ran} P^0 \gamma(\zeta)$;

(3) $\ker \gamma^*(z) P^0 \gamma(z) = \ker P^0 \gamma(\zeta)$, *i.e., the restriction of $\gamma^*(z)$ to $\operatorname{ran} P_0 \gamma(\zeta)$ is an injection. In particular,* $\dim \operatorname{ran} \gamma^*(z) P^0 \gamma(z) = \dim \operatorname{ran} P^0 \gamma(z)$.

Proof. (1) Recall that $P^0 = -i \lim_{\delta \to +0} \delta R^0(\varepsilon^0 + i\delta)$ in the weak operator topology. By (1.14b), for any $\delta > 0$ one has

$$\gamma(z) + (\varepsilon^0 + i\delta - z) R^0(\varepsilon^0 + i\delta)\gamma(z) = \gamma(\zeta) + (\varepsilon^0 + i\delta - \zeta) R^0(\varepsilon^0 + i\delta)\gamma(\zeta). \quad (4.1)$$

Multiplying (4.1) with δ and sending δ to 0 we arrive at

$$(\varepsilon^0 - z) P^0 \gamma(z) = (\varepsilon^0 - \zeta) P^0 \gamma(\zeta). \quad (4.2)$$

Now it is sufficient to recall that $\mathcal{N}_z = \operatorname{ran}\gamma(z)$ for all $z \in \operatorname{res}H^0$.

(2) Let $\phi \in \mathscr{H}^0 \cap \operatorname{dom}H_\Lambda$ and $\psi \in \mathcal{N}_z$. As H^0 and H_Λ are disjoint, $\phi \in \operatorname{dom}S$ and $S\phi = \varepsilon^0\phi$. There holds $(\varepsilon^0 - z)\langle\phi|\psi\rangle = \langle(S-\bar{z})\phi\,|\,\psi\rangle = \langle\phi\,|\,(S^* - z)\psi\rangle = 0$. Hence $\phi \perp \mathcal{N}_z$.

Conversely, let $\phi \in \mathscr{H}^0 \cap \mathcal{N}_z^\perp$. By (1.21d), $\gamma^*(z)\phi = 0$. As follows from the Krein resolvent formula (3.1), $(\varepsilon^0 - \bar{z})^{-1}\phi = R^0(\bar{z})\phi = R_\Lambda(\bar{z})\phi \in \operatorname{dom}H_\Lambda$. Hence, $\phi \in \operatorname{dom}H_\Lambda$, and the first equality is proved. The second equality follows immediately from the relations: (a) for any $\phi \in \mathscr{H}^0$ and $\psi \in \mathcal{N}_z$ one has $\langle\phi|\psi\rangle = \langle\phi, P^0\psi\rangle$, (b) $\mathcal{N}_z = \operatorname{ran}\gamma(z)$, (c) $\operatorname{ran}P^0\gamma(z) = \operatorname{ran}P^0\gamma(\zeta)$.

(3) Let $\gamma^*(z)P^0\gamma(\zeta)g = 0$. By (1.21d), $P^0\gamma(\zeta)g \perp \mathcal{N}_z$. According to (4.2), $P^0\gamma(\zeta)g \perp \mathcal{N}_\zeta$. It follows from the second equality in item (2) that $P^0\gamma(\zeta)g \perp \operatorname{ran}P^0\gamma(\zeta)$. Hence $P^0\gamma(\zeta)g = 0$. $\qquad\square$

The item (3) of lemma 4.1 can be generalized as follows.

Lemma 4.2. *Let ε_j, $j = 1,\ldots,m$, be distinct eigenvalues of H^0, P^j be orthoprojectors on the corresponding eigensubspaces and*

$$P := \sum_{j=1}^{m} P_j.$$

Then $(I - P)\gamma(z)$ is an injection for any $z \in \operatorname{res}H^0$.

Proof. Let $(I - P)\psi = 0$ where $\psi = \gamma(z)\phi$ for some $z \in \operatorname{res}H^0$, $\phi \in \mathscr{G}$. Then $\psi = P\psi \in \operatorname{dom}H^0$ and, therefore, $H^0\psi = z\psi$. Hence $\psi = 0$ and $\phi = 0$. $\qquad\square$

In what follows z_0 denotes a fixed number from $\operatorname{res}H^0$, $x_0 := \operatorname{Re}z_0$, $y_0 := \operatorname{Im}z_0$, $L := \gamma(z_0)$. Recall that L is a linear topological isomorphism on the deficiency subspace $\mathcal{N} := \mathcal{N}_{z_0} \subset \mathscr{H}$.

Since, by definition, $\gamma(z) = L + (z - z_0)R^0(z)L$ for any $z \in \operatorname{res}H^0$, the point ε^0 is either a regular point for γ or a simple pole with the residue

$$\operatorname{Res}[\gamma(z) : z = \varepsilon^0] = (z_0 - \varepsilon^0)P^0L. \tag{4.3}$$

Similarly, as $Q(z) = C + (z - x_0)L^*L + (z - z_0)(z - \bar{z}_0)L^*R^0(z)L$, with a bounded self-adjoint operator C (see proposition 1.20), the point ε^0 is either a regular point for Q or a simple pole with the residue:

$$\operatorname{Res}[Q(z) : z = \varepsilon^0] = -|\varepsilon^0 - z_0|^2 L^*P^0L. \tag{4.4}$$

From the equality $\|P^0L\phi\|^2 = \langle L^*P^0L\phi\,|\,\phi\rangle$ one easily sees that $\ker P^0L = \ker L^*P^0L$ (see also Lemma 4.1(3)). In particular, $P^0L = 0$ if and only if $L^*P^0L = 0$, and there are simple examples where $P^0L = 0$. Moreover, the following lemma holds.

Lemma 4.3. *Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be two Hilbert spaces and $A : \mathscr{H}_1 \to \mathscr{H}_2$ be a bounded linear operator. Then the two conditions below are equivalent:*

(1) $\operatorname{ran} A$ *is closed;*

(2) $\operatorname{ran} A^* A$ *is closed.*

In particular, $\operatorname{ran} P^0 L$ *is closed if and only if* $\operatorname{ran} L^* P^0 L$ *is closed.*

Proof. Condition (1) is satisfied if and only if there is a constant $c > 0$ such that $\|A\phi\| \geq c\|\phi\|$ for all $\phi \in (\ker A)^\perp$. On the other hand, condition (2) is satisfied if and only if there is a constant $c' > 0$ such that $\langle A^* A\phi \,|\, \phi \rangle \geq c'\|\phi\|^2$ for all $\phi \in (\ker A^* A)^\perp$. Since $\ker A^* A = \ker A$, we get the result. $\square$

Now we denote by $\mathscr{G}_r := \ker L^* P^0 L \subset \mathscr{G}$, $\mathscr{G}_1 := \mathscr{G}^\perp$. The orthoprojectors of $\mathscr{G}$ on $\mathscr{G}_r$ (respectively, on $\mathscr{G}_1$) are denoted by Π_r (respectively, by Π_1). If A is a bounded operator in $\mathscr{G}$, then we write $A_r := \Pi_r A \Pi_r$, and this will be considered as an operator in $\mathscr{G}_r$. If $z \in \operatorname{res} H^0$, then $\gamma_r(z)$ denotes the operator $(I - P^0)\gamma(z)\Pi_r$ acting from $\mathscr{G}_r$ to $\mathscr{H}$ (to avoid a confusion with the previous notation, we suppose without loss of generality $\mathscr{G} \neq \mathscr{H}$). Further, we denote by $\mathscr{H}_r$ the subspace $(I - P^0)\mathscr{H}$ and by H^0_r the part of H^0 in $\mathscr{H}_r$; clearly, $\varepsilon^0 \in \operatorname{res} H^0_r$, and both the mappings γ_r and Q_r have analytic continuation to ε^0. Finally, denote $\mathscr{G}_3 = \ker\left(Q_r(\varepsilon^0) - \Lambda_r\right)$, and $\mathscr{G}_2 = \mathscr{G}_r \ominus \mathscr{G}_3$.

Lemma 4.4. *There exists a closed symmetric densely defined restriction S_r of H^0_r such that γ_r is a Krein Γ-field for the triple $(S_r, H^0_r, \mathscr{G}_r)$, and Q_r is a Krein $\mathscr{Q}$-function associated with this triple and γ_r.*

Proof. We use proposition 1.18. Since P^0 and $R^0(z)$ commute for all $z \in \operatorname{res} H^0$, it is clear that γ_r satisfies the condition (1.14b). Further, z_0 belongs to $\operatorname{res} H^0_r$ and $\gamma_r(z_0) = (I - P_0)L\Pi_r$.

Let us show that the subspace $\mathscr{N}' := \operatorname{ran}\gamma_r(z_0)$ is closed. Let $(\phi_n) \in \mathscr{G}_r$ such that $\psi_n := (I - P^0)L\phi_n$ converge to some $\psi \in \mathscr{H}_r$. Since $\phi_n \in \mathscr{G}_r$, one has $L^* P^0 L\phi_n = 0$, hence $P^0 L\phi_n = 0$. On the other hand, $L\phi_n \in \mathscr{N}$ by definition of L. Denote the orthoprojector of $\mathscr{H}$ onto $\mathscr{N}$ by P, then we have $P\psi_n = L\phi_n$, hence $L\phi_n$ converge to $P\psi$. Therefore, the sequence $(L^* L\phi_n)$ converges to $L^* P\psi$ in $\mathscr{G}$. Since $L^* L$ is a linear topological automorphism of $\mathscr{G}$, there exists $\lim \phi_n$ and this limit belongs to $\mathscr{G}_r$ because $\mathscr{G}_r$ is closed. Thus, $\psi \in \mathscr{N}'$ and $\mathscr{N}'$ is closed.

By lemma 4.1(3), $\gamma_r(z_0)$ is injective. By the closed graph theorem, $\gamma_r(z_0)$ is a linear topological isomorphism of $\mathscr{G}_r$ onto $\mathscr{N}'$.

Now we show that $\mathscr{N}' \cap \operatorname{dom} H^0_r = 0$. It is sufficient to show that $\left((I - P^0)\mathscr{N}\right) \cap \operatorname{dom} H^0 = 0$. Let $\psi \in \left((I - P^0)\mathscr{N}\right) \cap \operatorname{dom} H^0$. As $\psi \in (I - P^0)\mathscr{N}$, we have $\psi = \phi - P^0\phi$ for some $\phi \in \mathscr{N}$. Since $\psi, P^0\phi \in \operatorname{dom} H^0$, $\phi \in \operatorname{dom} H^0$.

Hence $\phi = 0$ and $\psi = 0$. Thus, by proposition 1.18, there exists a closed symmetric densely defined restriction of H_r^0 such that γ_r is a Γ-field for the triple $(S_r, H_r^0, \mathscr{G}_r)$.

Since $Q(z) = C - iy_0 L^* L + (z - \bar{z}_0) L^* \gamma(z)$ with a bounded self-adjoint operator C in $\mathscr{G}$ (proposition 1.20), we have

$$
\begin{aligned}
Q_r(z) &= \Pi_r C \Pi_r - iy_0 \Pi_r L^* L \Pi_r + (z - \bar{z}_0) \Pi_r L^* \gamma(z) \Pi_r \\
&= \Pi_r C \Pi_r - iy_0 \Pi_r L^* (I - P^0) L \Pi_r \\
&\quad + (z - \bar{z}_0) \Pi_r L^* (I - P^0) \gamma(z) \Pi_r - iy_0 \Pi_r L^* P^0 L \Pi_r \\
&\quad + (z - \bar{z}_0) \Pi_r L^* P^0 \gamma(z) \Pi_r .
\end{aligned}
$$

Now we use the equations

$$
\Pi_r L^* P^0 L \Pi_r = 0 \qquad \Pi_r L^* P^0 \gamma(z) \Pi_r = 0 . \tag{4.5}
$$

The first one follows from definition of Π_r, to prove the second one we note that $\gamma(z) = L + (z - z_0) R^0(z) L$, therefore

$$
\Pi_r L^* P^0 \gamma(z) \Pi_r = \frac{\varepsilon^0 - z_0}{\varepsilon^0 - z} \Pi_r L^* P^0 L \Pi_r = 0 .
$$

From (4.5) we obtain

$$
Q_r(z) = C' - iy_0 \gamma_r^*(z_0) \gamma_r(z_0) + (z - \bar{z}_0) \gamma_r^*(z_0) \gamma_r(z) ,
$$

where $C' = \Pi_r C \Pi_r$ is a self-adjoint bounded operator in $\mathscr{G}_r$. Hence, Q_r is the Krein $\mathscr{Q}$-function associated with the Γ-field γ_r. $\qquad \square$

To prove the main result of the section we need the following lemma.

Lemma 4.5. *Let S be an analytic function in the disk $\mathbf{D} = \{z \in \mathbb{C} : |z| < r\}$ with values in the Banach space of all bounded linear operators $\mathbf{L}(\mathscr{G})$ such that there is a bounded inverse $S^{-1}(z)$ for all z from the punctured disk $\mathbf{D} \setminus \{0\}$ and the function $S^{-1}(z)$ is meromorphic. If $\ker S(0) = 0$, then $S_0 := S(0)$ has the bounded inverse (and, therefore, S^{-1} has an analytic continuation to the point 0 of the disk). If S_0 is self-adjoint and 0 is a pole at most of first order for $S^{-1}(z)$, then $\operatorname{ran} S_0$ is closed, i.e. there is a punctured neighborhood of 0 which has no point of $\operatorname{spec} S_0$.*

Proof. Consider the Laurent expansion

$$
S^{-1}(z) = \sum_{n=-m}^{\infty} T_n z^n .
$$

where m is a natural number. If $m \le 0$, the lemma is trivial. Suppose $m > 0$. Since $S(z)S^{-1}(z) = I$ for all z, we have $S_0 T_{-m} = 0$. Let $\ker S_0 = 0$, then $T_{-m} = 0$, and by recursion, $T_n = 0$ for all $n < 0$. Then $S_0 T_0 = T_0 S_0 = I$ and the first part of the lemma is proved.

Let now $m = 1$. Then $S_0 T_{-1} = 0$ and $T_{-1} S_1 + T_0 S_0 = I$, where $S_1 = S'(0)$. This implies $S_0 T_0 S_0 = S_0$. Let $x \in \operatorname{ran} S_0$, then $S_0 T_0 x = x$. Since $\operatorname{ran} S_0 \subset (\ker S_0)^\perp$, there is a linear operator $A : \operatorname{ran} S_0 \to \operatorname{ran} S_0$ such that $A S_0 x = x$ for all $x \in \operatorname{ran} S_0$. From $S_0 T_0 x = x$ we have $A = T_0$, i.e. A is bounded. Hence, there is $c > 0$ such that $\|x\| \le c \|S_0 x\|$ for all $x \in \operatorname{ran} S_0$ and hence for all $x \in (\ker S_0)^\perp$. $\qquad\square$

Remark 4.6. If 0 is a second order pole for $S^{-1}(z)$, then the range of S_0 can be non-closed. For example, let A be a self-adjoint operator in a Hilbert space $\mathscr{H}$ such that $\operatorname{ran} A$ is non-closed. Let $\mathscr{G} = \mathscr{H} \oplus \mathscr{H}$, and $S(z)$ is defined as follows

$$S(z) = \begin{bmatrix} A & z \\ z & 0 \end{bmatrix}.$$

Then

$$S^{-1}(z) = \frac{1}{z^2} \begin{bmatrix} 0 & z \\ z & -A \end{bmatrix}.$$

4.3 Description of eigensubspace

Theorem 4.7. *Let ε^0 be an isolated eigenvalue of H^0 and $\operatorname{ran} P^0 L$ be closed. Then the following assertions are mutually equivalent.*

(1) There exists a punctured neighborhood of ε^0 that contains no point of $\operatorname{spec} H_\Lambda$ (in particular, if $\varepsilon^0 \in \operatorname{spec} H_\Lambda$, then ε^0 is an isolated point in the spectrum of H_Λ).

(2) The operator $Q(z) - \Lambda$ has a bounded inverse for all z from a punctured neighborhood of ε^0.

(3) $\operatorname{ran} \left(Q_r(\varepsilon^0) - \Lambda_r \right)$ is closed.

(4) There is a punctured neighborhood of 0 which contains no point from the spectrum of the operator $Q_r(\varepsilon^0) - \Lambda_r$.

Let one of the condition (1)–(4) be satisfied. Then the eigensubspace $\mathscr{H}^0_\Lambda := \ker(H_\Lambda - \varepsilon^0)$ is the direct sum, $\mathscr{H}^0_\Lambda = \mathscr{H}_{\text{old}} \oplus \mathscr{H}_{\text{new}}$, where $\mathscr{H}_{\text{old}} = \mathscr{H}^0 \cap \operatorname{dom} H_\Lambda = \mathscr{H}^0 \cap \operatorname{dom} S$, $\mathscr{H}_{\text{new}} = \gamma_r(\varepsilon^0) \ker \left[Q_r(\varepsilon^0) - \Lambda_r \right]$ and $\dim \mathscr{H}^0 \ominus \mathscr{H}_{\text{old}} = \dim \mathscr{G} \ominus \mathscr{G}_r$. Therefore, $\varepsilon^0 \in \operatorname{spec} H_\Lambda$ if and only if at least one of the following two conditions is satisfied:

- $\mathscr{H}^0 \cap \operatorname{dom} H_\Lambda \neq \{0\}$,

- $\ker\left[Q_r(\varepsilon^0) - \Lambda_r\right] \neq \{0\}$.

Remark 4.8. Since $\mathscr{H}^0 \cap \operatorname{dom} H_\Lambda = \mathscr{H}^0 \cap \operatorname{dom} S$, the component $\mathscr{H}_{\text{old}}$ of $\ker(H_\Lambda - \varepsilon^0)$ is independent of Λ, i.e. this part is the same for all extensions of S disjoint to H^0. On the other hand, the component $\mathscr{H}_{\text{new}}$ depends on Λ.

Remark 4.9. Clearly, $\operatorname{ran} P^0 L$ is closed, if the deficiency index of S or $\dim \mathscr{H}^0$ are finite (this simple case is very important in applications of theorem 4.7). To show that the assumptions are essential for infinite deficiency indices, we provide here an example when the range of $P^0 L$ is not closed.

Let $\mathscr{H}_k = l^2(\mathbb{N})$ for $k = 0, 1, \ldots$ and let $(e_n^{(k)})_{n \geq 0}$ be the standard basis in $\mathscr{H}_k$: $e_n^{(k)} = (\delta_{mn})_{m \geq 0}$. Denote by H_k^0 the self-adjoint operator in $\mathscr{H}_k$ which is determined by $H_k^0 e_n^{(k)} = (n + 1/2)e_n^{(k)}$. Choose $a \in \mathscr{H}_0$ such that $\|a\| = 1$, $\langle a | e_0^{(0)} \rangle = 0$, $a \notin \mathscr{D}(H_0^0)$, and set $a^{(k)} = a$. Consider in $\mathscr{H}_k$ the one-dimensional subspace N_k generated by $e_0^{(k)} + (k+1)a^{(k)}$. Fix $z_0 \in \mathbb{C} \setminus \mathbb{R}$. By Proposition 1.18 there exists a symmetric restriction S_k of H_k^0 such that $\mathscr{N}_{z_0}(S_k) = N_k$. Let now $\mathscr{H} = \bigoplus \mathscr{H}_k$, $H^0 = \bigoplus H_k^0$, $S = \bigoplus S_k$. Then the eigensubspace $\mathscr{H}^0$ of H_0 corresponding to the eigenvalue $\varepsilon^0 = 1/2$ is the closed linear span of $(e_0^{(k)})$, $k = 0, 1, \ldots$, and $\mathscr{N}_{z_0}(S)$ is the closed linear span of $(e_0^{(k)} + (k+1)a^{(k)})$, $k = 0, 1, \ldots$. We can choose $\mathscr{G} := \mathscr{N}_{z_0}$, $\gamma(z_0) = L = I$ where I is the identical embedding of $\mathscr{N}_{z_0}$ into $\mathscr{H}$. It is clear, that the image of $P^0 L$ is the set M of all vectors x from $\mathscr{H}^0$ having the form $x = \sum \lambda_k e_0^{(k)}$ where $\sum (k+1)^2 |\lambda_k|^2 < \infty$. Obviously, M is dense in $\mathscr{H}^0$ but $M \neq \mathscr{H}^0$, hence M is not closed.

Proof of theorem 4.7. The equivalence $(1) \Leftrightarrow (2)$ follows from theorem 3.2, and the equivalence $(3) \Leftrightarrow (4)$ is trivial.

Let us prove the implication $(1) \Rightarrow (3)$. Choose $\mathscr{O} \in \mathscr{V}(\varepsilon^0)$ such that $Q(z) - \Lambda$ has a bounded inverse for all $z \in \mathscr{O} \setminus \{\varepsilon^0\}$ and for $z \in \mathscr{O} \setminus \{\varepsilon^0\}$ consider the mapping $T(z) = (z - \varepsilon^0)(Q(z) - \Lambda)$. Note that

- T has an analytic continuation to ε^0 by setting $T(\varepsilon^0) = -|\varepsilon^0 - z_0|^2 L^* P^0 L$, see Eq. (4.4), and

- T has a bounded inverse in $\mathscr{O} \setminus \{\varepsilon^0\}$.

Since the operator $L^* P_0 L$ has the closed range, we can apply a result of Kato ([87], Sections VII.1.3 and VII.3.1). According the mentioned result, there is a mapping V, $V \in \mathbf{K}(\mathscr{O}; \mathscr{G})$, such that the operator $V(z)T(z)V^{-1}(z)$ has the diagonal matrix representation with respect to the decomposition $\mathscr{G} = \mathscr{G}_1 \oplus \mathscr{G}_r$:

$$V^{-1}(z)T(z)V(z) = \begin{bmatrix} \hat{T}_{11}(z) & 0 \\ 0 & \hat{T}_{rr}(z) \end{bmatrix}. \tag{4.6}$$

Because the left-hand side of Eq. (4.6) has a bounded inverse for $z \in \mathcal{O} \setminus \{\varepsilon^0\}$, the same is true, in particular for the operator $S(z) := (z - \varepsilon^0)^{-1} \hat{T}_{rr}(z) = \Pi_r V^{-1}(z)[Q(z) - \Lambda]V(z)\Pi_r$ considered in the space $\mathcal{G}_r$.

Our next aim to prove that

$$\|S^{-1}(z)\| \leq c|z - \varepsilon^0|^{-1} \tag{4.7}$$

with a constant $c > 0$ for all z in a punctured neighborhood of ε^0. For this purpose we consider together with the decomposition $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_r$ of the space $\mathcal{G}$, the decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_r$, where $\mathcal{H}_1 = \mathcal{H}^0$, $\mathcal{H}_r = (I - P^0)\mathcal{H}^0$. In virtue of to the Krein resolvent formula (3.1),

$$(z - \varepsilon^0)R_\Lambda(z) = (z - \varepsilon^0)R^0(z) - (z - \varepsilon^0)^2 \gamma(z)T^{-1}(z)\gamma^*(\bar{z})$$
$$= (z - \varepsilon^0)R^0(z) - (z - \varepsilon^0)^2[\gamma(z)V(z)]V^{-1}(z)T^{-1}(z)V(z)[\gamma(\bar{z})V(\bar{z})]^*.$$

Represent the operator $\gamma(z)V(z)$ according to the above mentioned representations of $\mathcal{H}$ and $\mathcal{G}$ in the matrix form:

$$\gamma(z)V(z) = \begin{bmatrix} \hat{\gamma}_{11}(z) & \hat{\gamma}_{1r}(z) \\ \hat{\gamma}_{r1}(z) & \hat{\gamma}_{rr}(z) \end{bmatrix}. \tag{4.8}$$

Since $(z - \varepsilon^0)R_\Lambda(z)$ and $(z - \varepsilon^0)R^0(z)$ are analytic functions in a neighborhood of ε^0, all the matrix term in $[\gamma(z)V(z)]V^{-1}(z)T^{-1}(z)V(z)[\gamma(\bar{z})V(\bar{z})]^*$ are also analytic in the same neighborhood. In particular, we can chose $\mathcal{O}$ in such a way that the function

$$z \mapsto (z - \varepsilon^0)^2 \left(\hat{\gamma}_{r1}(z)\hat{T}_{11}^{-1}(z)\hat{\gamma}_{r1}^*(\bar{z}) + \hat{\gamma}_{rr}(z)\hat{T}_{rr}^{-1}(z)\hat{\gamma}_{rr}^*(\bar{z}) \right)$$

is analytic in $\mathcal{O}$. Since $\hat{T}_{11}(\varepsilon^0) \equiv -|z_0 - \varepsilon^0|^2 L^* P^0 L$ has a bounded inverse in $\mathcal{G}_1$, the function $\hat{T}_{11}^{-1}(z)$ is analytic in a neighborhood of ε^0. Therefore, we can chose $\mathcal{O}$ such that $(z - \varepsilon^0)^2 \hat{\gamma}_{rr}(z)\hat{T}_{rr}^{-1}(z)\hat{\gamma}_{rr}^*(\bar{z})$ is analytic in $\mathcal{O}$. Further $\hat{\gamma}_{rr}(\varepsilon^0) = \gamma_r(\varepsilon^0)$. In virtue of Lemma 4.4 and definition of the Γ-field, we can find a constant $c' > 0$ such that $\|\gamma_r(\varepsilon^0)g\| \geq c'\|g\|$ for all $g \in \mathcal{G}_r$. Therefore we can chose $\mathcal{O}$ so small that $\|\hat{\gamma}_{rr}(z)g\| \geq c''\|g\|$ for all $z \in \mathcal{O}$, $g \in \mathcal{G}_r$ with some $c'' > 0$. Since $\hat{\gamma}_{rr}^*(\bar{z})$ is an isomorphism of $\operatorname{ran} \gamma_r(\bar{z})$ on $\mathcal{G}_r$, we see that $(z - \varepsilon^0)^2 \hat{T}_{rr}^{-1}(z)$ is bounded in a neighborhood of ε^0. Hence, we obtain (4.7) in a punctured neighborhood of ε^0. By Theorem 3.13.3 from [76], $S^{-1}(z)$ has at point ε^0 a pole of the order ≤ 1. Therefore, $(1) \Rightarrow (3)$ by Lemma 4.5.

Now we prove $(4) \Rightarrow (2)$. Choose $\mathcal{O} \in \mathcal{V}(\varepsilon^0)$ such that $Q(z) - \Lambda$ has no spectrum in $\mathcal{O} \setminus \{\varepsilon^0\}$. Moreover, we can use again the representation (4.6). Since $V(z) = I + O(z - \varepsilon^0)$, the function $S(z) := \Pi_r V^{-1}(z)\Pi_r[Q(z) - \Lambda]\Pi_r V(z)\Pi_r$ has an analytic continuation at ε^0 with the value $S(\varepsilon^0) = Q_r(\varepsilon^0) - \Lambda_r$. To proceed further, we need the following auxiliary result.

Lemma 4.10. *The operator $S'(\varepsilon^0)$ is strictly positive on $\ker[Q_r(\varepsilon^0) - \Lambda_r]$.*

Proof of lemma 4.10. Since $V^{-1}(x) = V^*(x)$ for $x \in \mathscr{O} \cap \mathbb{R}$, for the derivative of S one has:

$$
\begin{aligned}
S'(\varepsilon^0) = &\Pi_r (V')^*(\varepsilon^0) \Pi_r [Q(\varepsilon^0) - \Lambda] \Pi_r \\
&+ \Pi_r [Q(\varepsilon^0) - \Lambda] \Pi_r V'(\varepsilon^0) \Pi_r + \Pi_r Q'(\varepsilon^0) \Pi_r
\end{aligned}
\tag{4.9}
$$

(note that $\Pi_r Q(\varepsilon^0)$ and $Q(\varepsilon^0) \Pi_r$ are well defined). Let now $\phi \in \ker[Q_r(\varepsilon^0) - \Lambda_r]$. Then we have from (4.9) that $\langle \phi | S'(\varepsilon^0) \phi \rangle = \langle \phi | Q'(\varepsilon^0) \phi \rangle$. Since $S'(\varepsilon^0)$ is a self-adjoint operator, we have that $S'(\varepsilon^0)\phi = Q'(\varepsilon^0)\phi$ on $\ker[Q_r(\varepsilon^0) - \Lambda_r]$. Therefore, by Lemma 4.4 and (1.22a),

$$
S'(\varepsilon^0)\phi = \gamma_r^*(\varepsilon^0)\gamma_r(\varepsilon^0)\phi \text{ for all } \phi \in \ker[Q_r(\varepsilon^0) - \Lambda_r], \tag{4.10}
$$

hence $S'(\varepsilon^0)$ is strictly positive on $\ker[Q_r(\varepsilon^0) - \Lambda_r]$. $\qquad\square$

To prove the required implication $(4) \Rightarrow (2)$, it is now sufficient to show that $S(z)$ has a bounded inverse in a punctured neighborhood of ε^0. Since $S(z)$ is analytic, it suffice to prove that the operator $J(z) := S(\varepsilon^0) + S'(\varepsilon^0)(z - \varepsilon^0)$ has a bounded inverse in a punctured neighborhood of ε^0 with the estimate $\|J(z)^{-1}\| \le c|z - \varepsilon^0|^{-1}$. For this purpose we represent $S'(\varepsilon^0)$ in the matrix form

$$
S'(\varepsilon^0) = \begin{bmatrix} S'_{22} & S'_{23} \\ S'_{32} & S'_{33} \end{bmatrix}
$$

according to the representation $\mathscr{G}_r = \mathscr{G}_2 \oplus \mathscr{G}_3$. Then J has the matrix representation

$$
J(z) = \begin{bmatrix} S_0 + (z - \varepsilon^0)S'_{22} & (z - \varepsilon^0)S'_{23} \\ (z - \varepsilon^0)S'_{32} & (z - \varepsilon^0)S'_{33}. \end{bmatrix}
$$

where $S_0 := S(\varepsilon^0)$. By the assumption of item (4), S_0 has a bounded inverse in $\mathscr{G}_2$, and by (4.10) the operator S'_{22} has a bounded inverse in $\mathscr{G}_3$. Now we use the Frobenius formula for the inverse of a block-matrix [78]:

$$
\begin{aligned}
&\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \\
&= \begin{bmatrix} [A_{11} - A_{12}A_{22}^{-1}A_{21}]^{-1} & A_{11}^{-1}A_{12}[A_{21}A_{11}^{-1}A_{12} - A_{22}]^{-1} \\ [A_{21}A_{11}^{-1}A_{12} - A_{22}]^{-1}A_{21}A_{11}^{-1} & [A_{22} - A_{21}A_{11}^{-1}A_{12}]^{-1} \end{bmatrix}
\end{aligned}
\tag{4.11}
$$

which is valid if all the inverse matrices on the right-hand side exist. Using (4.11) it is easy to see that $J^{-1}(z)$ exists for all z in a punctured neighborhood of ε^0 and obeys the estimate $\|J(z)^{-1}\| \le c|z - \varepsilon^0|^{-1}$ with some $c > 0$. Thus, the implication $(4) \Rightarrow (2)$ and, hence, the equivalence of all the items $(1) - (4)$ are proven.

Now suppose that the conditions of items (1) – (4) are satisfied. To determine the eigenspace $\mathscr{H}_\Lambda^0$ we find the orthoprojector P_Λ^0 on this space calculating the residue of the resolvent, $P_\Lambda^0 = -\operatorname{Res}[R_\Lambda(z) : z = \varepsilon^0] = P^0 + \operatorname{Res}[M(z) : z = \varepsilon_0]$, where

$$M(z) := \gamma(z)[Q(z) - \Lambda]^{-1}\gamma^*(\bar{z}).$$

Using the conditions of item (4), we find $\mathscr{O} \in \mathscr{V}(\varepsilon^0)$ and $V \in \mathbf{K}(\mathscr{O}, \mathscr{G})$ such that for z in $\mathscr{O} \setminus \{\varepsilon^0\}$

$$V^{-1}(z)[Q(z) - \Lambda]V(z) = \begin{bmatrix} S_1(z) & 0 \\ 0 & S_r(z) \end{bmatrix},$$

according to the decomposition $\mathscr{G} = \mathscr{G}_1 \oplus \mathscr{G}_r$ where S_1 and S_r have the following properties: S_r is analytic in $\mathscr{O}$ with $S_r(\varepsilon^0) = Q_r(\varepsilon^0) - \Lambda_r$ and

$$S_1(z) = -|\varepsilon^0 - z_0|^2 \frac{L^* P^0 L}{z - \varepsilon^0} + F_1(z), \text{ where } F_1 \text{ is analytic in } \mathscr{O}. \tag{4.12}$$

Using Lemma 4.10, we find a function $W \in \mathbf{K}(\mathscr{O}, \mathscr{G}_r)$ such that for z in $\mathscr{O} \setminus \{\varepsilon^0\}$ one has

$$W^{-1}(z)S_r(z)W(z) = \begin{bmatrix} S_2(z) & 0 \\ 0 & S_3(z) \end{bmatrix},$$

according to the decomposition $\mathscr{G}_r = \mathscr{G}_2 \oplus \mathscr{G}_3$ where S_2 and S_3 have the properties:

$$\ker S_2(\varepsilon^0) = 0 \text{ and } S_2(\varepsilon^0)\phi = [Q_r(\varepsilon^0) - \Lambda_r]\phi \text{ for } \phi \in \mathscr{G}_2, \tag{4.13}$$

S_3 is analytic in $\mathscr{O}$ and has the form $S_3(z) = (z - \varepsilon^0)T(z)$ where $T_0 := T(\varepsilon^0)$ is a strictly positive operator in $\mathscr{G}_3$. $\tag{4.14}$

Denote now

$$U(z) := V(z)\begin{bmatrix} I_1 & 0 \\ 0 & W(z) \end{bmatrix},$$

where the matrices are decomposed according to the representation $\mathscr{G} = \mathscr{G}_1 \oplus \mathscr{G}_r$ and I_1 is the identity operator on $\mathscr{G}_1$. Further, denote $\hat{Q}(z) = U^{-1}(z)[Q(z) - \Lambda]U(z)$, $\hat{\gamma}(z) = \gamma(z)U(z)$, then $M(z) = \hat{\gamma}(z)\hat{Q}^{-1}(z)\hat{\gamma}^*(\bar{z})$, and for $z \in \mathscr{O} \setminus \{\varepsilon^0\}$ one has

$$\hat{Q}^{-1}(z) = \begin{bmatrix} S_1^{-1}(z) & 0 & 0 \\ 0 & S_2^{-1}(z) & 0 \\ 0 & 0 & S_3^{-1}(z) \end{bmatrix}.$$

An important property of $\hat{\gamma}$ we need is follows

$$\hat{\gamma}(z) = \frac{z_0 - \varepsilon^0}{z - \varepsilon^0}P^0 LU(z) + (I - P^0)\gamma(z)U(z), \tag{4.15}$$

and $(I - P^0)\gamma$ is analytic in $\mathcal{O}$. Represent M as the sum $M(z) = A_1(z) + A_2(z) + A_3(z)$, where $A_j(z) = \hat{\gamma}(z)\Pi_j S_j^{-1}(z)\Pi_j \hat{\gamma}^*(\bar{z})$; here Π_j denote the orthoprojectors of $\mathcal{G}$ onto $\mathcal{G}_j$, $j = 1, 2, 3$.

It is clear from (4.12)–(4.15) that at the point $z = \varepsilon^0$, the function $A_j(z)$ has a pole at most of j-th order. Let

$$A_j(z) = A_j^{(-j)}(z - \varepsilon^0)^{-j} + A_j^{(-j+1)}(z - \varepsilon^0)^{-j+1} + \ldots$$

be the Laurent expansion for A_j at the point ε^0. According to the definition of $A_j(z)$ and formulas (4.12)–(4.15) we have

$$A_j^{(-j)} = C_j B_j C_j^*, \quad A_j^{(-j+1)} = C_j B_j D_j^* + D_j B_j C_j^* + C_j B_j' C_j^*,$$

where

$$C_j = (z_0 - \varepsilon^0)P^0 L\Pi_j, \quad B_1 = |\varepsilon^0 - z_0|^{-2}(\Pi_1 L^* P^0 L\Pi_1)^{-1},$$
$$B_2 = (\Pi_2 S(\varepsilon^0)\Pi_2)^{-1}, \quad B_3 = (\Pi_3 T_0 \Pi_3)^{-1},$$

and B_j', C_j, D_j are some bounded operators (we need no concrete form of them). By definition of the spaces $\mathcal{G}_j$, we have $\Pi_j L^* P^0 L\Pi_j = 0$ for $j = 2, 3$, and hence, $P^0 L\Pi_j = 0$ for the same j's. As a result we have that $A_2(z)$ has no pole at $z = \varepsilon^0$, i.e.,

$$\text{Res}\,[A_2(z) : z = \varepsilon^0] = 0, \tag{4.16}$$

and $A_3(z)$ has at this point a pole at least of first order. Using (4.15) and taking into consideration $P^0 L\Pi_3 = 0$, we obtain

$$\begin{aligned}
\text{Res}\,[A_3(z) : z = \varepsilon^0] =: P_3 &= (I - P^0)\gamma(\varepsilon^0)\Pi_3 T_0^{-1}\Pi_3 \gamma^*(\varepsilon^0)(I - P^0) \\
&= \gamma_r(\varepsilon^0)\Pi_3 T_0^{-1}\Pi_3 \gamma_r^*(\varepsilon^0).
\end{aligned} \tag{4.17}$$

Now we have according to (4.12) and (4.15)

$$\text{Res}\,[A_1(z) : z = \varepsilon^0] =: -P_1 = -P^0 L\Pi_1(\Pi_1 L^* P^0 L\Pi_1)^{-1}\Pi_1 L^* P^0. \tag{4.18}$$

As a result, we have from (4.16), (4.17), and (4.18) $P_\Lambda^0 = P^0 - P_1 + P_3$.

Eq. (4.18) shows that P_1 is an orthoprojector with $\text{ran}\,P_1 \subset \text{ran}\,P^0$. Therefore, $P^0 - P_1$ is an orthoprojector on a subspace of $\mathcal{H}^0$. Eq. (4.17) shows that $\text{ran}\,P_3 \subset \text{ran}(I - P^0)$, therefore $(P^0 - P_1)P_3 = 0$. Since P_3 is self-adjoint, $P_3(P^0 - P_1) = 0$. Using $(P_\Lambda^0)^2 = P_\Lambda^0$ we see that $P_3^2 = P_3$, hence P_3 is an orthoprojector and $P_3 \perp P^0$.

By Lemma 4.1, $\text{ran}(P^0 - P_1) = \mathcal{H}^0 \cap \text{dom}\,H_\Lambda \equiv \mathcal{H}_{\text{old}}$. The relation $\text{ran}\,P_3 = \gamma_r(\varepsilon^0)\ker\left[Q_r(\varepsilon^0) - \Lambda_r\right] \equiv \mathcal{H}_{\text{new}}$ follows from (4.17) and the definition of $\mathcal{G}_3$. Theorem 4.7 is proved. $\square$

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