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Singular values and trace formulae for resolvent power differences of self-adjoint elliptic operators

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Devoted to my parents Yury M. Lotoreichik and Evgeniya L. Ratner, and to the memory of my school teacher of mathematics Aleksei K. Vinogradov (1951–2010).

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Abstract

In the present thesis a unified functional analytic approach to the treatment of self-adjoint elliptic operators with Dirichlet, Neumann, Robin, and more general self-adjoint boundary conditions on bounded and unbounded domains is provided. Moreover, Schrödinger operators on couplings of exterior and interior domains with transmission boundary conditions are considered. In particular, Schrödinger operators with δ'-interactions on hypersurfaces are rigorously introduced.

The key results in the thesis are Schatten-von Neumann estimates for the resolvent power differences of self-adjoint elliptic operators corresponding to the same differential expression and to distinct boundary conditions. Schatten-von Neumann estimates for the resolvent power differences of elliptic operators have a long history, starting in the middle of the 20th century with the seminal contributions by Povzner and Birman, followed by Grubb. In this thesis certain new estimates with faster convergence of singular values are obtained. The proofs of these estimates rely on Krein-type resolvent formulas, asymptotics of eigenvalues of the Laplace-Beltrami operator on the boundary and certain considerations of algebraic nature.

A question of special interest, in connection with scattering theory, is the trace class property of the analyzed resolvent power differences, which implies the existence and completeness of the wave operators. In the special case, that the resolvent power differences are in the trace class, formulae for their traces are given.

Zusammenfassung

In der vorliegenden Dissertation wird eine Methode zur Behandlung von selbstadjungierten elliptischen Operatoren mit Dirichlet-, Neumann-, Robin- und allgemeineren selbstadjungierten Randbedingungen auf beschränkten und unbeschränkten Gebieten vorgeschlagen, die auf der Erweiterungstheorie symmetrischer Operatoren basiert. Außerdem werden Schrödinger-Operatoren auf äußeren und inneren Gebieten betrachtet, die durch Transmissionsbedingungen gekoppelt sind. Als Spezialfall werden Schrödinger-Operatoren mit δ'-Interaktionen auf Hyperflächen rigoros eingeführt.

Die entscheidenden Resultate der Dissertation sind Schatten-von Neumann Abschätzungen der Resolventpotenzdifferenzen von selbstadjungierten elliptischen Operatoren, die mit einem Differentialausdruck und verschiedenen Randbedingungen assoziiert sind. Schatten-von Neumann Abschätzungen von Resolventpotenzdifferenzen elliptischer Operatoren haben eine lange Geschichte, die in der Mitte des 20. Jahrhunderts mit den grundlegenden Artikeln von Povzner, Birman und Grubb anfing. In dieser Dissertation sind bestimmte neue Abschätzungen mit schnellerer Konvergenz von Singulärwerten enthalten. Die Beweise dieser Abschätzungen basieren auf der Kreinschen Resolventidentität, dem asymptotischen Verhalten der Eigenwerten des Laplace-Beltrami Operators auf dem Rand und einigen algebraischen Beobachtungen.

Eine Frage von speziellem Interesse, mit Verbindung zur Streutheorie, ist die Spurklasseeigenschaft der analysierten Resolventenpotenzdifferenzen, welche die Existenz und Vollständingkeit der Welleoperatoren impliziert. In dem Spezialfall, dass die Resolventenpotenzdifferenzen in der Spurklasse liegen, werden Formeln für ihre Spuren gegeben.

Contents

Chapter 1

Introduction

Partial differential equations play a major role in natural sciences and pure mathematics. The present thesis is concerned with the fields of operator theory and analysis of partial differential equations, more particular, spectral theory of elliptic differential operators. In many situations it is useful and natural to associate linear operators with differential expressions, e.g. in quantum mechanics, where the observables are often self-adjoint partial differential operators in Hilbert spaces, and their spectral properties are related to the behavior of the quantum mechanical systems.

The evolution of a quantum system is governed by the time-dependent Schrödinger equation. The behavior for large times of the solutions of this equation is the subject of analysis in scattering theory. From the functional analytic point of view mathematical scattering theory can be considered as perturbation theory of self-adjoint operators on the continuous spectrum. The main objects are the wave operators and the corresponding scattering operator, which relates "initial" and "final" characteristics of the process directly, bypassing its consideration for finite times. The initial step in the solution of a scattering problem usually consists in establishing the existence and completeness of the wave operators. One possible way to show the existence and completeness of the wave operators for a pair of self-adjoint operators is to prove that the difference of some integer powers of their resolvents belongs to the trace class ideal.

In the present thesis the author provides a unified approach to the treatment of self-adjoint elliptic operators with Dirichlet, Neumann, Robin, and more general self-adjoint boundary conditions on bounded and unbounded domains. The key results in the thesis are Schatten-von Neumann estimates for the resolvent power differences of self-adjoint elliptic operators corresponding to one differential expression and to distinct boundary conditions. Schatten-von Neumann estimates for the resolvent power differences of elliptic operators have a long history, starting in the middle of the 20th century with the seminal contributions by Povzner [P53] and Birman [B62], followed by Grubb [G84]. In the thesis certain new estimates with faster convergence of singular values are presented. A question of special interest, in connection with scattering theory, is the trace class property of the analyzed resolvent power differences, which implies the existence and completeness of the wave operators. In the special case that the resolvent power differences are in the trace class, we provide formulae for their traces.

The main content of the thesis is divided into four chapters, namely: Chapter 2 with preliminary material, Chapter 3 on elliptic operators on domains with compact boundaries, Chapter 4 on Schrödinger operators with couplings of interior and exterior domains, and Chapter 5 on Robin Laplacians on a half-space. The introduction is further organized into three parts corresponding to the material presented in Chapters 3-5.

The main results of the thesis are partially reflected in five publications [BLL+10, BLL12, BLL12a, BLL12b, LR12] jointly with Jussi Behrndt, Matthias Langer, Igor Lobanov, Igor Popov, and Jonathan Rohleder.

1.1 Elliptic operators on domains with compact boundaries

In Chapter 3 we deal with self-adjoint realizations of a symmetric elliptic differential expression on a bounded or unbounded domain with a compact smooth boundary subject to Dirichlet, Neumann, Robin and more general boundary conditions. We explain the main results of Chapter 3 with the help of the Laplace differential expression. In the body of the thesis the statements are formulated and proved for a second-order uniformly elliptic differential expression with certain assumptions on the coefficients.

Let $\Omega \subset \mathbb{R}^n$ be a bounded or unbounded domain with a compact C^∞-smooth boundary $\partial\Omega$. We denote by $-\Delta_{\mathrm{D}}$ and $-\Delta_{\mathrm{N}}$ the self-adjoint Dirichlet and Neumann Laplacians on Ω. For a bounded self-adjoint operator B, which acts in the Hilbert space $L^2(\partial\Omega)$, we define the operator $-\Delta_{[B]}$ as

$$(1.1.1)\qquad \begin{aligned} -\Delta_{[B]} &:= -\Delta f \\ \mathrm{dom}\,\big(-\Delta_{[B]}\big) &:= \big\{ f \in H^{3/2}(\Omega)\colon \Delta f \in L^2(\Omega),\ Bf|_{\partial\Omega} = \partial_\nu f|_{\partial\Omega}\big\}, \end{aligned}$$

where $H^{3/2}(\Omega)$ is the fractional Sobolev space on Ω of order $3/2$, $f|_{\partial\Omega}$ is the trace of f on the boundary and $\partial_\nu f|_{\partial\Omega}$ is the trace of the normal derivative of f with the normal pointing outwards. Using the second Green's identity it is not difficult to show that the operator $-\Delta_{[B]}$ is symmetric, whereas in order to show self-adjointness of $-\Delta_{[B]}$ certain tools are required.

Our key tools are the notion of quasi boundary triples, and the associated γ-fields and Weyl functions. This allows us to prove the Krein-type formula

$$(1.1.2)\qquad (-\Delta_{[B]}-\lambda)^{-1}-(-\Delta_{\mathrm{N}}-\lambda)^{-1}=\gamma(\lambda)\big(I-BM(\lambda)\big)^{-1}B\gamma(\overline{\lambda})^*,$$

where $\lambda\in\rho(-\Delta_{[B]})\cap\rho(-\Delta_{\mathrm{N}})$. In this formula, the γ-field $\gamma(\lambda)\colon L^2(\partial\Omega)\to L^2(\Omega)$ is the solution operator for the boundary value problem

$$(1.1.3)\qquad \begin{aligned}(-\Delta-\lambda)f&=0,\quad \text{in } \Omega,\\ \partial_\nu f|_{\partial\Omega}&=\varphi,\quad \text{on } \partial\Omega,\end{aligned}$$

and the Weyl function $M(\lambda)\colon L^2(\partial\Omega)\to L^2(\partial\Omega)$ is the corresponding Neumann-to-Dirichlet map, which maps φ into the Dirichlet trace of the solution of the problem (1.1.3). As an intermediate step in the proof of formula (1.1.2) we get self-adjointness of the operator $-\Delta_{[B]}$.

The main results of Chapter 3 are related to Schatten-von Neumann estimates for resolvent power differences of the operators $-\Delta_{\mathrm{D}}$, $-\Delta_{\mathrm{N}}$ and $-\Delta_{[B]}$. We recall that the singular values $s_k(T)$ of a compact operator T are the eigenvalues of the positive operator $(T^*T)^{1/2}$ arranged in non-increasing order and counted with their multiplicities. If the singular values satisfy $s_k(T)=O(k^{-1/p})$ as $k\to\infty$ with some $p>0$, then we write $T\in\mathfrak{S}_{p,\infty}$. The class $\mathfrak{S}_{p,\infty}$ is called the *weak Schatten-von Neumann class* of order p. In particular, an operator $T\in\mathfrak{S}_{p,\infty}$ with $p\in(0,1)$ belongs to the *trace class*, which means that $\{s_k(T)\}_{k=1}^\infty\in\ell^1(\mathbb{N})$.

According to the results, proved by Povzner [P53], Birman [B62] and Grubb [G84, G84a], for all $m\in\mathbb{N}$,

$$(1.1.4)\qquad (-\Delta_{\mathrm{D}}-\lambda)^{-m}-(-\Delta_{\mathrm{N}}-\lambda)^{-m}\in\mathfrak{S}_{\frac{n-1}{2m},\infty},$$

holds, and, moreover, this estimate is optimal. In the special case, that B is a multiplication operator with a real-valued function $\beta\in C^\infty(\partial\Omega)$, it was also proved in [G84, G84a] that

$$(1.1.5)\qquad (-\Delta_{\mathrm{D}}-\lambda)^{-m}-(-\Delta_{[\beta]}-\lambda)^{-m}\in\mathfrak{S}_{\frac{n-1}{2m},\infty},$$

and that this estimate is also optimal. In the thesis the estimates (1.1.4) and (1.1.5) are generalized to the pairs $\{-\Delta_{[B]},-\Delta_{\mathrm{N}}\}$ and $\{-\Delta_{[B]},-\Delta_{\mathrm{D}}\}$.

We emphasize that for the pair $\{-\Delta_{[B]}, -\Delta_{\mathrm{N}}\}$, even in the case of a multiplication operator B, known results were not optimal. As it is shown in Chapter 3, in this case singular values converge slightly faster, which in view of the sharpness of the estimates (1.1.4) and (1.1.5) is a new phenomenon. Namely, we prove that

$$
\begin{aligned}
&(-\Delta_{[B]} - \lambda)^{-m} - (-\Delta_{\mathrm{N}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1},\infty}, \\
&(-\Delta_{[B]} - \lambda)^{-m} - (-\Delta_{\mathrm{D}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}.
\end{aligned}
\tag{1.1.6}
$$

In this sense the operator $-\Delta_{[B]}$ is closer to $-\Delta_{\mathrm{N}}$. These estimates are especially important in the case of exterior domains, for which scattering problems make sense. Clearly, for a sufficiently large number m we get $\frac{n-1}{2m+1} < 1$ and $\frac{n-1}{2m} < 1$. Thus for such m the resolvent power differences in (1.1.6) are trace class operators and by the Birman-Kato criterion [Y92] the wave operators for the pairs $\{-\Delta_{[B]}, -\Delta_{\mathrm{N}}\}$ and $\{-\Delta_{[B]}, -\Delta_{\mathrm{D}}\}$ exist and are complete, see Section 3.3 for the details.

Our proofs of the estimates in (1.1.6) rely on the formula (1.1.2), on elliptic regularity theory and on the spectral asymptotics of the Laplace-Beltrami operator on $\partial\Omega$.

It is worth mentioning that for B_1 and B_2 such that $B_1 - B_2 \in \mathfrak{S}_{\frac{n-1}{q},\infty}$ with some $q > 0$ we get even a better estimate

$$
(-\Delta_{[B_2]} - \lambda)^{-m} - (-\Delta_{[B_1]} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+q+1},\infty}.
\tag{1.1.7}
$$

In the special case, that the resolvent power differences in (1.1.6) and (1.1.7) are in the trace class, we provide formulae for their traces extending the work of Carron [Ca02] to more general boundary conditions. In particular, for the pair $\{-\Delta_{[B]}, -\Delta_{\mathrm{N}}\}$ this formula has the form

$$
\operatorname{tr}\big((-\Delta_{[B]}-\lambda)^{-m}-(-\Delta_{\mathrm{N}}-\lambda)^{-m}\big) = \operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(\big(I-BM(\lambda)\big)^{-1}B\frac{d}{d\lambda}M(\lambda)\Big)\right).
$$

Note that on the left-hand side the trace of an operator in $L^2(\Omega)$ appears, whereas on the right-hand side the trace of an operator in $L^2(\partial\Omega)$ is computed. In this sense we reduce the trace to the boundary. In Sturm-Lioville theory an analogous reduction of perturbation determinants was given already sixty years ago by Jost and Pais in [JP51].

See Section 3.4 for further references and historical comments. The results of Chapter 3 are mainly contained in the works of the author [BLL+10, BLL12, BLL12b].

1.2 Schrödinger operators with δ and δ'-potentials supported on compact hypersurfaces

In Chapter 4 we study self-adjoint realizations of the Schrödinger differential expression $-\Delta + V$ in the Hilbert space $L^2(\mathbb{R}^n)$ with certain coupling (transmission) boundary conditions on a compact C^∞-smooth, closed hypersurface. In the introduction we present our results in the special important case $V \equiv 0$.

We deal with a compact C^∞-smooth closed hypersurface $\Sigma \subset \mathbb{R}^n$ which separates the Euclidean space $\mathbb{R}^n, n \geq 2$, into an interior bounded domain $\Omega_{\rm i}$ and an exterior unbounded domain $\Omega_{\rm e}$. By $-\Delta_{\rm free}$ we denote the usual self-adjoint Laplacian in $L^2(\mathbb{R}^n)$ with $\mathrm{dom}(-\Delta_{\rm free}) = H^2(\mathbb{R}^n)$ and by $-\Delta_{\rm N,i,e}$ we denote the direct sum of the self-adjoint Neumann Laplacians on the domains $\Omega_{\rm i}$ and $\Omega_{\rm e}$.

Usually the Schrödinger operator with a δ-interaction of a strength $\alpha \in L^\infty(\Sigma; \mathbb{R})$ supported on Σ is defined via the closed semi-bounded sesquilinear form

$$\mathfrak{t}_{\delta,\alpha}[f,g] := (\nabla f, \nabla g)_{L^2(\mathbb{R}^n;\mathbb{C}^n)} - (\alpha f|_\Sigma, g|_\Sigma)_{L^2(\Sigma)}, \quad \mathrm{dom}\,\mathfrak{t}_{\delta,\alpha} := H^1(\mathbb{R}^n).$$

This way of definition is used in many papers. We refer the reader to Brasche, Exner, Kuperin and Šeba [BEKS94] and the review paper [E08] by Exner for more details and further references, see also Section 4.6 for historical comments.

The definition via the sesquilinear form does not immediately lead to an explicit characterization of the operator domain of the underlying self-adjoint operator, whereas the regularity of the functions in the operator domain plays an important role in many applications. In the thesis the author suggests another way of definition of the Schrödinger operator with a δ-interaction supported on Σ of strength α, where the action and the domain are specified explicitly. Set

$$H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma) := \big\{ f = f_{\rm i} \oplus f_{\rm e} \in H^{3/2}(\Omega_{\rm i}) \oplus H^{3/2}(\Omega_{\rm e}) : \Delta f_{\rm j} \in L^2(\Omega_{\rm j}),\ {\rm j} = {\rm i}, {\rm e} \big\}.$$

Then the operator $-\Delta_{\delta,\alpha}$ can be defined as

(1.2.1)

$$-\Delta_{\delta,\alpha} := -\Delta f_{\rm i} \oplus \Delta f_{\rm e},$$

$$\mathrm{dom}(-\Delta_{\delta,\alpha}) := \left\{ f = f_{\rm i} \oplus f_{\rm e} \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma) : \begin{array}{c} f_{\rm i}|_\Sigma = f_{\rm e}|_\Sigma =: f|_\Sigma \\ \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma + \partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma = \alpha f|_\Sigma \end{array} \right\},$$

where $f_\mathrm{i}|_\Sigma$, $f_\mathrm{e}|_\Sigma$ are the traces of $f = f_\mathrm{i} \oplus f_\mathrm{e}$ from both sides of Σ and $\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma$, $\partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma$ are the traces of the normal derivatives of f from both sides of Σ with the normals pointing outwards Ω_i and Ω_e, respectively. Roughly speaking, the domain of the operator $-\Delta_{\delta,\alpha}$ consists of functions with coinciding traces from both sides of Σ and with a jump of the normal derivative, which is connected with the usual trace via the function α. It follows from the second Green's identity that the operator $-\Delta_{\delta,\alpha}$ is symmetric. For the proof of self-adjointness we need certain tools.

Our key tools are similar as in the case of single domains in Chapter 3. We introduce a γ-field $\widetilde{\gamma}$, which is in this case the single-layer potential, and the corresponding Weyl function $\widetilde{M}$, which is an analogue of the Neumann-to-Dirichlet map. This allows us to prove the Krein-type formula

$$(-\Delta_{\delta,\alpha} - \lambda)^{-1} - (-\Delta_{\mathrm{free}} - \lambda)^{-1} = \widetilde{\gamma}(\lambda)\big(I - \alpha\widetilde{M}(\lambda)\big)^{-1}\alpha\widetilde{\gamma}(\overline{\lambda})^{*}. \tag{1.2.2}$$

As an intermediate step in the proof of this formula we get self-adjointness of the operator $-\Delta_{\delta,\alpha}$. We also prove in Chapter 4 that the operator $-\Delta_{\delta,\alpha}$ and the operator corresponding to the form $\mathfrak{t}_{\delta,\alpha}$ coincide, which relates our approach to the previously known one.

Furthermore, we obtain spectral estimates of the type (1.1.6) for the pairs $\{-\Delta_{\mathrm{free}}, -\Delta_{\delta,\alpha}\}$ and $\{-\Delta_{\mathrm{N,i,e}}, -\Delta_{\delta,\alpha}\}$. Namely, for all $m \in \mathbb{N}$,

$$\begin{aligned} &(-\Delta_{\delta,\alpha} - \lambda)^{-m} - (-\Delta_{\mathrm{free}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1},\infty}, \\ &(-\Delta_{\delta,\alpha} - \lambda)^{-m} - (-\Delta_{\mathrm{N,i,e}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}. \end{aligned} \tag{1.2.3}$$

In this sense the operator $-\Delta_{\delta,\alpha}$ is closer to the free Laplacian than to the decoupled Neumann Laplacian. In particular, as a consequence of these estimates the wave operators for the pair $\{-\Delta_{\delta,\alpha}, -\Delta_{\mathrm{free}}\}$ exist and are complete in all space dimensions. Our proofs of $\mathfrak{S}_{p,\infty}$-estimates in the case of δ-interactions are similar to the proofs in the case of single domains without coupling. We use the formula (1.2.2), elliptic regularity theory and the asymptotics of Laplace-Beltrami operator on Σ.

As a certain addition we provide trace formulae in the case that the resolvent power differences in (1.2.3) are in the trace class. In these formulae the trace of the resolvent power difference acting in $L^2(\mathbb{R}^n)$ is reduced to the trace of a certain operator acting in $L^2(\Sigma)$. For a more general differential expression $-\Delta + V$ we assume some smoothness of V in the neighborhood of Σ in order to prove the estimates (1.2.3).

In the thesis also δ'-interactions on hypersurfaces are encompassed. Since δ'-interactions are more singular, their treatment is more involved. Some particular results in the case of Σ being a sphere are known, see Antoine, Gesztesy and Shabani [AGS87], Shabani [Sh88], where the separation of variables is the main tool of analysis. Development of a general approach to the treatment of Schrödinger operators with δ'-interactions supported on hypersurfaces was posed by Pavel Exner as an unsolved problem in the review paper [E08]. We provide two ways for the definition of these operators. As we show, one can define for a boundedly invertible real-valued function $\beta\colon \Sigma \to \mathbb{R}$ the Schrödinger operator with a δ'-interaction supported on Σ of the strength β via the closed, semi-bounded sesquilinear form

$$\begin{aligned}\mathfrak{t}_{\delta',\beta}[f,g] &:= \big(\nabla f_{\rm i}, \nabla g_{\rm i}\big)_{L^2(\Omega_{\rm i};\mathbb{C}^n)} + \big(\nabla f_{\rm e}, \nabla g_{\rm e}\big)_{L^2(\Omega_{\rm e};\mathbb{C}^n)} - \\ &\qquad - \big(\beta^{-1}(f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma), g_{\rm e}|_\Sigma - g_{\rm i}|_\Sigma\big)_{L^2(\Sigma)} \\ \operatorname{dom} \mathfrak{t}_{\delta',\beta} &:= H^1(\Omega_{\rm i}) \oplus H^1(\Omega_{\rm e}).\end{aligned}$$

In this definition the domain of the underlying self-adjoint operator is not easily visible. As the second way, we propose to define Schrödinger operator with a δ'-interaction explicitly via its action and domain

$$\begin{aligned}-\Delta_{\delta',\beta} &:= -\Delta f_{\rm i} \oplus \Delta f_{\rm e} \\ \operatorname{dom}(-\Delta_{\delta',\beta}) &:= \left\{ f = f_{\rm i} \oplus f_{\rm e} \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma)\colon \begin{matrix} f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma = \beta \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma \\ \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma + \partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma = 0 \end{matrix} \right\}.\end{aligned}$$

Roughly speaking, the domain of the operator $-\Delta_{\delta',\beta}$ consists of functions with coinciding normal derivatives on Σ and with the jump of the usual traces, which is connected with the normal derivative via the function β. In order to see that the operator $-\Delta_{\delta',\beta}$ is self-adjoint, we follow our abstract methods with γ-fields and Weyl functions. Furthermore, we connect the two proposed definitions by showing that the self-adjoint operator $-\Delta_{\delta',\beta}$ coincides with the self-adjoint operator corresponding to the form $\mathfrak{t}_{\delta',\beta}$.

We obtain estimates of the type (1.2.3) also for the pairs $\{-\Delta_{\rm free}, -\Delta_{\delta',\beta}\}$ and $\{-\Delta_{\rm N,i,e}, -\Delta_{\delta',\beta}\}$. As we show, for all $m \in \mathbb{N}$,

$$\begin{aligned}(-\Delta_{\delta',\beta} - \lambda)^{-m} - (-\Delta_{\rm free} - \lambda)^{-m} &\in \mathfrak{S}_{\frac{n-1}{2m},\infty}, \\ (-\Delta_{\delta',\beta} - \lambda)^{-m} - (-\Delta_{\rm N,i,e} - \lambda)^{-m} &\in \mathfrak{S}_{\frac{n-1}{2m+1},\infty}.\end{aligned} \tag{1.2.4}$$

In this sense the operator $-\Delta_{\delta',\beta}$ is closer to the decoupled Neumann Laplacian than to the free Laplacian. In particular, as a consequence of these results the wave operators for the pair $\{-\Delta_{\delta',\beta}, -\Delta_{\rm free}\}$ exist and are complete in all space dimensions. For the trace class resolvent power differences in (1.2.4) we provide corresponding trace formulae.

See Section 4.6 for further references and historical comments. The results of Chapter 4 are mainly contained in the joint work of the author [BLL12a].

1.3 Robin Laplacians on a half-space

In Chapter 5 we are concerned with the half-space

$$\mathbb{R}^n_+ := \{(x, x')^{\mathrm{T}} \colon x \in \mathbb{R}^{n-1}, x' \in \mathbb{R}_+\}$$

with the boundary $\partial\mathbb{R}^n_+$. Our main focus is the usual Robin Laplace operator defined as

$$\begin{aligned} -\Delta_{[\beta]} &:= -\Delta f, \\ \mathrm{dom}(-\Delta_{[\beta]}) &:= \big\{ f \in H^{3/2}(\mathbb{R}^n_+) \colon \Delta f \in L^2(\mathbb{R}^n_+), \beta f|_{\partial\mathbb{R}^n_+} = \partial_\nu f|_{\partial\mathbb{R}^n_+} \big\}, \end{aligned}$$

where $f|_{\partial\mathbb{R}^n_+}$ and $\partial_\nu f|_{\partial\mathbb{R}^n_+}$ denote the trace of f on the boundary of the half-space and the trace of the normal derivative of f with the normal pointing outwards, respectively, which are connected by the real-valued function $\beta \in L^\infty(\partial\mathbb{R}^n_+)$. In order to show that the operator $-\Delta_{[\beta]}$ is self-adjoint in $L^2(\mathbb{R}^n_+)$ we use our abstract approach with a modification in the arguments due to the non-compactness of the boundary. As a particular case we also treat the self-adjoint Neumann Laplacian $-\Delta_{\mathrm{N}}$ on the half-space.

Let β_1 and β_2 be real-valued bounded functions on $\partial\mathbb{R}^n_+$. The resolvent difference

$$(-\Delta_{[\beta_2]} - \lambda)^{-1} - (-\Delta_{[\beta_1]} - \lambda)^{-1} \tag{1.3.1}$$

is in general non-compact. Indeed, if we take two positive constants $b_1 \neq b_2$ and assume that $\beta_1 \equiv b_1$ and $\beta_2 \equiv b_2$, then a simple calculation shows that the essential spectra

$$\sigma_{\mathrm{ess}}(-\Delta_{[b_1]}) = \big[-b_1^2, +\infty\big) \quad \text{and} \quad \sigma_{\mathrm{ess}}(-\Delta_{[b_2]}) = \big[-b_2^2, +\infty\big)$$

of the corresponding Robin Laplacians are distinct and thus the operator in (1.3.1) is evidently non-compact.

The first result is concerned with the assumption on $\beta_2 - \beta_1$ sufficent for the compactness of the resolvent difference in (1.3.1). Namely, if for all $\varepsilon > 0$ the condition

$$\mu\big\{x \in \partial\mathbb{R}^n_+ \colon \big|\beta_2(x) - \beta_1(x)\big| \geq \varepsilon\big\} < \infty$$

holds with μ being the standard Lebesgue measure, then the resolvent difference in (1.3.1) is compact. The proof of the compactness of the resolvent difference in (1.3.1) relies on the compact embedding of $H^1(\Omega)$ into $L^2(\Omega)$ for a domain Ω of finite measure with a smooth boundary. As a particular case, we get the condition on β for compactness of the resolvent difference of $-\Delta_{[\beta]}$ and $-\Delta_{\mathrm{N}}$. Using recent results by Malamud and Neidhardt [MN11] we get that under this condition the absolutely continuous parts of the self-adjoint operators $-\Delta_{[\beta]}$ and $-\Delta_{\mathrm{N}}$ are unitarily equivalent.

Another question is to find sufficient conditions on β_1 and β_2 such that for $m \in \mathbb{N}$ the resolvent power difference

$$(-\Delta_{[\beta_2]} - \lambda)^{-m} - (-\Delta_{[\beta_1]} - \lambda)^{-m} \tag{1.3.2}$$

belongs to a $\mathfrak{S}_{p,\infty}$-class of the same order as the first resolvent power difference in (1.1.6). It turns out to be sufficient to require boundedness of all the partial derivatives of β_1 and β_2 up to order $2m-1$ and to assume that $\beta_2 - \beta_1$ is compactly supported, or at least that $n > 4m$ and

$$\beta_2 - \beta_1 \in L^{\frac{n-1}{2m+1}}(\partial\mathbb{R}^n_+).$$

Under these assumptions the resolvent power difference (1.3.2) belongs to the class $\mathfrak{S}_{\frac{n-1}{2m+1},\infty}$. Here we rely on a result by Cwikel [Cw77] on $\mathfrak{S}_{p,\infty}$-estimates of integral operators. The cases of slower decaying $\beta_2 - \beta_1$ are also considered in Chapter 5. The results for high resolvent powers complement papers by Birman [B62], Gorbachuk and Kutovoi [GorK82], Derkach and Malamud [DM91], where only the first powers of resolvents were considered. Moreover, for compactly supported $\beta_2 - \beta_1$ and for some non-compactly supported $\beta_2 - \beta_1$ we provide corresponding trace formulae for the resolvent power difference in (1.3.2). The results of Chapter 5 are partially contained in the work of the author [LR12].

Chapter 2

Preliminaries

2.1 Classes of operator ideals

In this section we introduce the notion of classes of operator ideals. Further we define singular values and related (weak) Schatten-von Neumann classes of operator ideals. Two important technical lemmas are provided for Schatten-von Neumann estimates of resolvent power differences of self-adjoint operators. Throughout this section let $\mathcal{H}$ and $\mathcal{K}$ be separable Hilbert spaces. Denote by $\mathfrak{S}_\infty(\mathcal{H},\mathcal{K})$ the closed subspace of compact operators in $\mathcal{B}(\mathcal{H},\mathcal{K})$; if $\mathcal{H}=\mathcal{K}$, we simply write $\mathfrak{S}_\infty(\mathcal{H})$.

2.1.1 Abstract classes of operator ideals

We define classes of operator ideals along the lines of [Pi87].

Definition 2.1. Suppose that for every pair of Hilbert spaces $\mathcal{H}$, $\mathcal{K}$ we are given a subset $\mathfrak{A}(\mathcal{H},\mathcal{K})$ of $\mathfrak{S}_\infty(\mathcal{H},\mathcal{K})$. The set

$$\mathfrak{A} := \bigcup_{\mathcal{H},\mathcal{K} \text{ Hilbert spaces}} \mathfrak{A}(\mathcal{H},\mathcal{K})$$

is said to be a *class of operator ideals* if the following conditions are satisfied:

(i) the rank-one operators $x \mapsto (x,u)v$ are in $\mathfrak{A}(\mathcal{H},\mathcal{K})$ for all $u \in \mathcal{H}$, $v \in \mathcal{K}$;

(ii) $A + B \in \mathfrak{A}(\mathcal{H},\mathcal{K})$ for $A, B \in \mathfrak{A}(\mathcal{H},\mathcal{K})$;

(iii) $CAB \in \mathfrak{A}(\mathcal{H}_1,\mathcal{K}_1)$ for $A \in \mathfrak{A}(\mathcal{H},\mathcal{K})$, $B \in \mathcal{B}(\mathcal{H}_1,\mathcal{H})$, $C \in \mathcal{B}(\mathcal{K},\mathcal{K}_1)$.

Moreover, we write $\mathfrak{A}(\mathcal{H})$ for $\mathfrak{A}(\mathcal{H},\mathcal{H})$.

If $\mathfrak{A}$ is a class of operator ideals, then the sets $\mathfrak{A}(\mathcal{H},\mathcal{K})$ are *two-sided operator ideals* for every pair $\mathcal{H}$, $\mathcal{K}$; for the latter notion see also, e.g. [GK69, Pi80]. For two classes of operator ideals $\mathfrak{A}$, $\mathfrak{B}$ we define the product

$$\mathfrak{A}\cdot\mathfrak{B} := \big\{T\colon \text{there exist } A\in\mathfrak{A}, B\in\mathfrak{B} \text{ so that } T = AB\big\}$$

and the adjoint of $\mathfrak{A}$ by

$$\mathfrak{A}^* := \big\{A^*\colon A\in\mathfrak{A}\big\}.$$

These sets are again classes of operator ideals; see [Pi87].

Let H and K be linear operators in a separable Hilbert space $\mathcal{H}$ and assume that $\rho(H)\cap\rho(K)\neq\varnothing$. We are aiming to investigate operator ideal properties of the difference of the m-th powers of the resolvents,

$$(H-\lambda)^{-m}-(K-\lambda)^{-m},\qquad \lambda\in\rho(H)\cap\rho(K),\ m\in\mathbb{N}.$$

Recall that for two elements a and b of some non-commutative algebra the following formula holds:

$$a^m - b^m = \sum_{k=0}^{m-1} a^{m-k-1}\big(a-b\big)b^k. \tag{2.1.1}$$

Substituting a and b by the resolvents of H and K, respectively, and setting

$$T_{m,k}(\lambda) := (H-\lambda)^{-(m-k-1)}\Big((H-\lambda)^{-1}-(K-\lambda)^{-1}\Big)(K-\lambda)^{-k} \tag{2.1.2}$$

for $\lambda\in\rho(H)\cap\rho(K)$, $m\in\mathbb{N}$ and $k=0,1,\dots,m-1$, we conclude from (2.1.1) that

$$(H-\lambda)^{-m}-(K-\lambda)^{-m} = \sum_{k=0}^{m-1} T_{m,k}(\lambda) \tag{2.1.3}$$

holds for all $\lambda\in\rho(H)\cap\rho(K)$ and $m\in\mathbb{N}$. In the next lemma we show that $(H-\lambda)^{-m}-(K-\lambda)^{-m}$ belongs to the ideal $\mathfrak{A}(\mathcal{H})$ for all $\lambda\in\rho(H)\cap\rho(K)$ if all the operators $T_{m,0}(\lambda_0), T_{m,1}(\lambda_0),\dots,T_{m,m-1}(\lambda_0)$ belong to $\mathfrak{A}(\mathcal{H})$ for some $\lambda_0\in\rho(H)\cap\rho(K)$.

Lemma 2.2. *Let H and K be linear operators in $\mathcal{H}$ such that $\rho(H)\cap\rho(K)\neq\varnothing$. Let $m\in\mathbb{N}$ and let $T_{m,k}$ be as in (2.1.2). Assume that $T_{m,k}(\lambda_0)\in\mathfrak{A}(\mathcal{H})$ for some $\lambda_0\in\rho(H)\cap\rho(K)$ and all $k=0,\dots,m-1$. Then*

$$(H-\lambda)^{-m}-(K-\lambda)^{-m}\in\mathfrak{A}(\mathcal{H})$$

holds for all $\lambda\in\rho(H)\cap\rho(K)$.

Proof. For $\lambda\in\rho(H)\cap\rho(K)$ define

$$E_\lambda := I+(\lambda-\lambda_0)(H-\lambda)^{-1} \quad\text{and}\quad F_\lambda := I+(\lambda-\lambda_0)(K-\lambda)^{-1}. \tag{2.1.4}$$

Clearly, E_λ commutes with $(H-\lambda_0)^{-1}$ and F_λ commutes with $(K-\lambda_0)^{-1}$. The resolvent identity implies that

$$E_\lambda(H-\lambda_0)^{-1}=(H-\lambda)^{-1} \quad\text{and}\quad (K-\lambda_0)^{-1}F_\lambda=(K-\lambda)^{-1},$$

and hence also

$$E_\lambda^l(H-\lambda_0)^{-l}=(H-\lambda)^{-l} \quad\text{and}\quad (K-\lambda_0)^{-l}F_\lambda^l=(K-\lambda)^{-l} \tag{2.1.5}$$

for all $l\in\mathbb{N}$. Set $D_1(\lambda):=(H-\lambda)^{-1}-(K-\lambda)^{-1}$, $\lambda\in\rho(H)\cap\rho(K)$. Then (2.1.4) and (2.1.5) imply that

$$E_\lambda D_1(\lambda_0)F_\lambda=(H-\lambda)^{-1}F_\lambda-E_\lambda(K-\lambda)^{-1}=D_1(\lambda). \tag{2.1.6}$$

For $k=0,1,2\dots,m-1$ we obtain from (2.1.5) and (2.1.6) that

$$\begin{aligned}
T_{m,k}(\lambda)&=(H-\lambda)^{-(m-k-1)}E_\lambda D_1(\lambda_0)F_\lambda(K-\lambda)^{-k}\\
&=E_\lambda^{m-k-1}(H-\lambda_0)^{-(m-k-1)}E_\lambda D_1(\lambda_0)F_\lambda(K-\lambda_0)^{-k}F_\lambda^k\\
&=E_\lambda^{m-k}(H-\lambda_0)^{-(m-k-1)}D_1(\lambda_0)(K-\lambda_0)^{-k}F_\lambda^{k+1}\\
&=E_\lambda^{m-k}T_{m,k}(\lambda_0)F_\lambda^{k+1}
\end{aligned}$$

holds for all $\lambda\in\rho(H)\cap\rho(K)$. By the assumption we have $T_{m,k}(\lambda_0)\in\mathfrak{A}(\mathcal{H})$ and hence we conclude $T_{m,k}(\lambda)\in\mathfrak{A}(\mathcal{H})$ for $k=0,\dots,m-1$. This together with (2.1.3) yields that

$$(H-\lambda)^{-m}-(K-\lambda)^{-m}=\sum_{k=0}^{m-1}T_{m,k}(\lambda)\in\mathfrak{A}(\mathcal{H}),\quad \lambda\in\rho(H)\cap\rho(K).$$

□

2.1.2 Singular values, $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$-classes

Recall that the *singular values* (or *s-numbers*) $s_k(A)$, $k = 1, 2, \ldots$, of a compact operator $A \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K})$ are defined as the eigenvalues $\lambda_k(|A|)$ of the non-negative compact operator $|A| = (A^*A)^{\frac{1}{2}} \in \mathfrak{S}_\infty(\mathcal{H})$, which are enumerated in non-increasing order and with multiplicities taken into account. Note that for a non-negative operator $A \in \mathfrak{S}_\infty(\mathcal{H})$ the eigenvalues $\lambda_k(A)$ and singular values $s_k(A)$, $k = 1, 2, \ldots$, coincide. Let $A \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K})$ and assume that $\mathcal{H}$ and $\mathcal{K}$ are infinite-dimensional Hilbert spaces. Then there exist orthonormal systems $\{\varphi_1, \varphi_2, \ldots\}$ and $\{\psi_1, \psi_2, \ldots\}$ in $\mathcal{H}$ and $\mathcal{K}$, respectively, such that A admits the *Schmidt expansion*

$$A = \sum_{k=1}^{\infty} s_k(A)(\,\cdot\,, \varphi_k)\psi_k. \tag{2.1.7}$$

It follows, for instance, from (2.1.7) and the corresponding expansion for $A^* \in \mathfrak{S}_\infty(\mathcal{K}, \mathcal{H})$ that the singular values of A and A^* coincide: $s_k(A) = s_k(A^*)$ for $k = 1, 2, \ldots$; see, e.g. [GK69, II.§2.2]. Moreover, if $\mathcal{G}$ and $\mathcal{L}$ are separable Hilbert spaces, $B \in \mathcal{B}(\mathcal{G}, \mathcal{H})$ and $C \in \mathcal{B}(\mathcal{K}, \mathcal{L})$, then the estimates

$$s_k(AB) \le \|B\| s_k(A) \quad \text{and} \quad s_k(CA) \le \|C\| s_k(A), \qquad k = 1, 2, \ldots, \tag{2.1.8}$$

hold. If, in addition, $B \in \mathfrak{S}_\infty(\mathcal{G}, \mathcal{H})$ we have

$$s_{m+n-1}(AB) \le s_m(A) s_n(B), \qquad m, n = 1, 2 \ldots. \tag{2.1.9}$$

The proofs of the inequalities (2.1.8) and (2.1.9) are the same as in [GK69, II.§2.1 and §2.2], where these facts are shown for operators acting in the same space.

Recall that the *Schatten–von Neumann ideals* $\mathfrak{S}_p(\mathcal{H}, \mathcal{K})$ are defined by

$$\mathfrak{S}_p(\mathcal{H}, \mathcal{K}) := \left\{ A \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K}) \colon \sum_{k=1}^{\infty} (s_k(A))^p < \infty \right\}, \qquad p > 0.$$

Besides the standard Schatten–von Neumann ideals also the *weak Schatten-von Neumann ideals*

$$\mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K}) := \left\{ A \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K}) \colon s_k(A) = O(k^{-1/p}),\ k \to \infty \right\}, \quad p > 0,$$

will play an important role later on. The sets

$$\mathfrak{S}_p := \bigcup_{\mathcal{H}, \mathcal{K}} \mathfrak{S}_p(\mathcal{H}, \mathcal{K}) \quad \text{and} \quad \mathfrak{S}_{p,\infty} := \bigcup_{\mathcal{H}, \mathcal{K}} \mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K}).$$

are classes of operator ideals in the sense of Definition 2.1.

We refer the reader to [GK69, III.§7 and III.§14] and [Si05, Chapter 2] for a detailed study of the classes $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$. We list only some basic and well-known properties, which will be useful for us. It follows from $s_k(A) = s_k(A^*)$ that $\mathfrak{S}_p^* = \mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}^* = \mathfrak{S}_{p,\infty}$ hold.

Lemma 2.3. *Let $p, q, r, s, t > 0$. Then the following statements are true:*

(i) $\mathfrak{S}_{p,\infty} \cdot \mathfrak{S}_{q,\infty} = \mathfrak{S}_{r,\infty}$ *with* $p^{-1} + q^{-1} = r^{-1}$, *or, equivalently* $\mathfrak{S}_{\frac{1}{s},\infty} \cdot \mathfrak{S}_{\frac{1}{t},\infty} = \mathfrak{S}_{\frac{1}{s+t},\infty}$.

(ii) $\mathfrak{S}_p \cdot \mathfrak{S}_q = \mathfrak{S}_r$ *with* $p^{-1} + q^{-1} = r^{-1}$, *or, equivalently* $\mathfrak{S}_{\frac{1}{s}} \cdot \mathfrak{S}_{\frac{1}{t}} = \mathfrak{S}_{\frac{1}{s+t}}$;

(iii) $\mathfrak{S}_p \subset \mathfrak{S}_{p,\infty}$ *and* $\mathfrak{S}_{p',\infty} \subset \mathfrak{S}_p$ *for* $p' < p$.

Proof. In order to verify (i) let $p, q > 0$ and set $r := \frac{pq}{p+q}$. Let $A \in \mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K})$ and $B \in \mathfrak{S}_{q,\infty}(\mathcal{G}, \mathcal{H})$, that is, the inequalities $s_n(A) \le c_a n^{-1/p}$ and $s_n(B) \le c_b n^{-1/q}$, $n \in \mathbb{N}$, hold with some constants $c_a, c_b > 0$. From (2.1.9) we obtain

$$s_{2n}(AB) \le s_{2n-1}(AB) \le s_n(A)s_n(B) \le \frac{c_a c_b}{n^r} \le \frac{2^r c_a c_b}{(2n)^r} \le \frac{2^r c_a c_b}{(2n-1)^r},$$

which implies $AB \in \mathfrak{S}_{r,\infty}(\mathcal{G}, \mathcal{K})$. In order to show equality, let $A \in \mathfrak{S}_{r,\infty}(\mathcal{H}, \mathcal{K})$ with Schmidt expansion

$$A = \sum_k s_k(A)(\,\cdot\,, \varphi_k)\psi_k.$$

Define operators $B\colon \mathcal{H} \to \mathcal{K}$ and $C\colon \mathcal{H} \to \mathcal{H}$ by

$$B = \sum_k \big(s_k(A)\big)^{\frac{q}{p+q}}(\,\cdot\,, \varphi_k)\psi_k, \qquad C = \sum_k \big(s_k(A)\big)^{\frac{p}{p+q}}(\,\cdot\,, \varphi_k)\varphi_k.$$

The relations $A = BC$, $B \in \mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K})$, $C \in \mathfrak{S}_{q,\infty}(\mathcal{H}, \mathcal{H})$ show that $A \in \mathfrak{S}_{p,\infty} \cdot \mathfrak{S}_{q,\infty}$. The same arguments as in (i) can be used to show (ii). The inclusions in (iii) are trivial. $\square$

The *trace class* of the class of *nuclear operators* $\mathfrak{S}_1$ plays an important role later on. The trace of a compact operator $K \in \mathfrak{S}_1(\mathcal{H})$ is defined as

$$\operatorname{tr} K := \sum_{k=1}^{\infty} \lambda_k(K),$$

where $\lambda_k(K)$ are the eigenvalues of K and the sum converges absolutely. It is well-known (see, e.g. [GK69, §III.8]) that for $K_1, K_2 \in \mathfrak{S}_1(\mathcal{H})$

$$\operatorname{tr}(K_1 + K_2) = \operatorname{tr} K_1 + \operatorname{tr} K_2 \tag{2.1.10}$$

holds. Moreover, for $K_1 \in \mathcal{B}(\mathcal{H}, \mathcal{K})$ and $K_2 \in \mathcal{B}(\mathcal{K}, \mathcal{H})$ such that $K_1K_2 \in \mathfrak{S}_1(\mathcal{K})$ and $K_2K_1 \in \mathfrak{S}_1(\mathcal{H})$ one has

$$\operatorname{tr}(K_1K_2) = \operatorname{tr}(K_2K_1). \tag{2.1.11}$$

The following two lemmas will be used in the next chapters to show that certain resolvent power differences of elliptic operators are in some classes $\mathfrak{S}_{p,\infty}$ or $\mathfrak{S}_p$.

Lemma 2.4. *Let $\mathcal{H}$ and $\mathcal{G}$ be some Hilbert spaces. Let H and K be linear operators in $\mathcal{H}$ and assume that for some $\lambda_0 \in \rho(H) \cap \rho(K)$ there exist operators $F_1 \in \mathcal{B}(\mathcal{G}, \mathcal{H})$ and $F_2 \in \mathcal{B}(\mathcal{H}, \mathcal{G})$ such that*

$$(H - \lambda_0)^{-1} - (K - \lambda_0)^{-1} = F_1F_2. \tag{2.1.12}$$

Let $a > 0$ and $b_1, b_2 \geq 0$ be such that $a \leq b_1 + b_2$ and set $b := b_1 + b_2 - a$. Moreover, let $r \in \mathbb{N} \cup \{\infty\}$ and assume that for $k = 0, 1, \ldots, r-1$

$$(K - \lambda_0)^{-k}F_1 \in \mathfrak{S}_{\frac{1}{ak+b_1},\infty} \quad \text{and} \quad F_2(K - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak+b_2},\infty} \tag{2.1.13}$$

holds. Then for $l = 1, 2, \ldots, r$ and all $\lambda \in \rho(H) \cap \rho(K)$

$$(H - \lambda)^{-l} - (K - \lambda)^{-l} \in \mathfrak{S}_{\frac{1}{al+b},\infty}. \tag{2.1.14}$$

The statement of the lemma is true with $\mathfrak{S}_{p,\infty}$-classes replaced by $\mathfrak{S}_p$-classes.

Proof. We prove the statement by induction with respect to l. Using the factorization in (2.1.12), the assumptions in (2.1.13) with $k = 0$ and Lemma 2.3 (i) we obtain that

$$(H - \lambda_0)^{-1} - (K - \lambda_0)^{-1} = F_1F_2 \in \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{b_2},\infty} = \mathfrak{S}_{\frac{1}{b_1+b_2},\infty} = \mathfrak{S}_{\frac{1}{a+b},\infty}.$$

Now Lemma 2.2 with $m = 1$ implies that

$$(H - \lambda)^{-1} - (K - \lambda)^{-1} \in \mathfrak{S}_{\frac{1}{a+b}}$$

for all $\lambda \in \rho(H) \cap \rho(K)$, i.e. (2.1.14) is true for $l = 1$.

For the induction step fix $m \in \mathbb{N}$, $2 \leq m \leq r$, and assume that (2.1.14) is satisfied for all $l = 1, 2, \ldots, m-1$. Let $T_{m,k}$ be as in (2.1.2), and define for $k = 0, 1, \ldots, m-1$

$$D_k := (H - \lambda_0)^{-k} - (K - \lambda_0)^{-k}.$$

Note that $D_0 = 0$. Let us rewrite $T_{m,k}(\lambda_0)$ with $k = 0, 1, \ldots, m-1$ as sums of two operators

(2.1.15)

$$\begin{aligned} T_{m,k}(\lambda_0) =& (H - \lambda_0)^{-(m-k-1)} F_1 F_2 (K - \lambda_0)^{-k} \\ =& D_{m-k-1} F_1 F_2 (K - \lambda_0)^{-k} + (K - \lambda_0)^{-(m-k-1)} F_1 F_2 (K - \lambda_0)^{-k}. \end{aligned}$$

Note that the first summand is missing when $k = m-1$. By the assumption (2.1.13) we have

$$\begin{aligned} &F_1 \in \mathfrak{S}_{\frac{1}{b_1},\infty}, \quad F_2 (K - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak+b_2},\infty}, \\ &(K - \lambda_0)^{-(m-k-1)} F_1 \in \mathfrak{S}_{\frac{1}{a(m-k-1)+b_1},\infty}, \end{aligned}$$

for $k = 0, 1, \ldots, m-1$. By the induction assumption we also have

$$D_{m-k-1} \in \mathfrak{S}_{\frac{1}{a(m-k-1)+b},\infty}$$

for $k = 0, 1, \ldots, m-2$ and and hence we obtain by Lemma 2.3 (i) that the first summand in (2.1.15) is in the class

$$\mathfrak{S}_{\frac{1}{a(m-k-1)+b},\infty} \cdot \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{ak+b_2},\infty} = \mathfrak{S}_{\frac{1}{am+2b},\infty} \subset \mathfrak{S}_{\frac{1}{am+b},\infty},$$

where we used that $b \geq 0$. The second summand in (2.1.15) is in the class

$$\mathfrak{S}_{\frac{1}{a(m-k-1)+b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{ak+b_2},\infty} = \mathfrak{S}_{\frac{1}{am+b},\infty}.$$

Hence $T_{m,k}(\lambda_0) \in \mathfrak{S}_{\frac{1}{am+b},\infty}$ for all $k = 0, 1, \ldots, m-1$. Now Lemma 2.2 implies the validity of (2.1.14) for $l = m$. The induction process yields that the statement is true for every $l = 1, 2, \ldots, r$. Similarly with the help of Lemma 2.3 (ii) one can show the analogous result for $\mathfrak{S}_p$-classes. $\square$

Remark 2.5. In the proof of the last lemma we used the algebraic identity

$$a^m - b^m = \sum_{k=0}^{m-1} \Big((a^{m-k-1} - b^{m-k-1})(a-b)b^k + b^{m-k-1}(a-b)b^k \Big)$$

valid for any two elements a and b of a non-commutative algebra. In our case $a = (H-\lambda)^{-1}$ and $b = (K-\lambda)^{-1}$. In applications to elliptic operators we take for K a self-adjoint elliptic operator with known smoothing properties of its resolvent, while smoothing properties of the resolvent of the operator H can be unknown and they may be weaker, see Section 3.3 and Section 4.4.

Lemma 2.6. *Let $\mathcal{H}$ and $\mathcal{G}$ be some Hilbert spaces. Let H, K and L be linear operators in $\mathcal{H}$. Assume that for some $\lambda_0 \in \rho(H)\cap\rho(K)\cap\rho(L)$ there exist operators $F_1 \in \mathcal{B}(\mathcal{G},\mathcal{H})$ and $F_2 \in \mathcal{B}(\mathcal{H},\mathcal{G})$ such that*

$$(H-\lambda_0)^{-1} - (K-\lambda_0)^{-1} = F_1F_2. \tag{2.1.16}$$

Let $a > 0$ and $b_1, b_2 \geq 0$ be such that $a \leq b_1 + b_2$ and set $b := b_1 + b_2 - a$. Let $r \in \mathbb{N}\cup\{\infty\}$ and assume also that for $k = 0, 1, \ldots, r-1$

$$(L-\lambda_0)^{-k}F_1 \in \mathfrak{S}_{\frac{1}{ak+b_1},\infty} \quad \text{and} \quad F_2(L-\lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak+b_2},\infty}. \tag{2.1.17}$$

Moreover, assume that for $k = 1, 2, \ldots, r-1$

$$\begin{aligned} &(H-\lambda_0)^{-k} - (L-\lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak},\infty}, \\ &(K-\lambda_0)^{-k} - (L-\lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak},\infty}. \end{aligned} \tag{2.1.18}$$

Then for $l = 1, 2, \ldots, r$ and all $\lambda \in \rho(H)\cap\rho(K)$

$$(H-\lambda)^{-l} - (K-\lambda)^{-l} \in \mathfrak{S}_{\frac{1}{al+b},\infty}. \tag{2.1.19}$$

The statement of the lemma is true with $\mathfrak{S}_{p,\infty}$-classes replaced by $\mathfrak{S}_p$-classes.

Proof. By (2.1.16), (2.1.17) with $k = 0$, and the equality $b = b_1 + b_2 - a$ we get

$$(H-\lambda_0)^{-1} - (K-\lambda_0)^{-1} = F_1F_2 \in \mathfrak{S}_{\frac{1}{b_1},\infty}\cdot\mathfrak{S}_{\frac{1}{b_2},\infty} = \mathfrak{S}_{\frac{1}{a+b},\infty},$$

where we used Lemma 2.3 (i). Then by Lemma 2.2

$$(H-\lambda)^{-1} - (K-\lambda)^{-1} \in \mathfrak{S}_{\frac{1}{a+b},\infty}$$

for all $\lambda \in \rho(H)\cap\rho(K)$. Thus the statement is true for $l = 1$.

Let us fix $l \in \mathbb{N}$, $2 \leq l \leq r$, and define for $k = 0, 1, \ldots, l-1$ the differences of k-th resolvent powers

$$\begin{aligned} D_k &:= (H-\lambda_0)^{-k} - (L-\lambda_0)^{-k}, \\ G_k &:= (K-\lambda_0)^{-k} - (L-\lambda_0)^{-k}. \end{aligned}$$

Note that $D_0 = G_0 = 0$. First we rewrite each of the operators $T_{l,0}(\lambda_0)$ and $T_{l,l-1}(\lambda_0)$ in (2.1.2) as a sum of two operators

$$T_{l,0}(\lambda_0) = S_1 + S_2 \quad \text{and} \quad T_{l,l-1}(\lambda_0) = S_3 + S_4,$$

where $S_1 = D_{l-1}F_1F_2$, $S_2 = (L-\lambda_0)^{-(l-1)}F_1F_2$, $S_3 = F_1F_2G_{l-1}$ and $S_4 = F_1F_2(L-\lambda_0)^{-(l-1)}$. By the assumptions (2.1.17), (2.1.18), the equality $b = b_1 + b_2 - a$ and by Lemma 2.3 (i) we obtain that

$$\begin{aligned}
S_1 &\in \mathfrak{S}_{\frac{1}{a(l-1)},\infty} \cdot \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{b_2},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty}.\\
S_2 &\in \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{a(l-1)+b_2},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty},\\
S_3 &\in \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{b_2},\infty} \cdot \mathfrak{S}_{\frac{1}{a(l-1)},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty},\\
S_4 &\in \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{a(l-1)+b_2},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty}.
\end{aligned}$$

We conclude that

$$T_{l,0}(\lambda_0),\, T_{l,l-1}(\lambda_0) \in \mathfrak{S}_{\frac{1}{al+b},\infty}. \tag{2.1.20}$$

Further we rewrite the operator $T_{l,k}(\lambda_0)$ in (2.1.2) with $k \in \mathbb{N}$, $1 \le k \le l-2$, as a linear combination of four operators

$$T_{l,k}(\lambda_0) := S_5 + S_6 + S_7 - S_8,$$

where

$$\begin{aligned}
S_5 = D_{l-k-1}F_1F_2G_k, &\quad S_6 = (L-\lambda_0)^{-(l-k-1)}F_1F_2G_k,\\
S_7 = D_{l-k-1}F_1F_2(L-\lambda_0)^{-k}, &\quad S_8 = (L-\lambda_0)^{-(l-k-1)}F_1F_2(L-\lambda_0)^{-k}.
\end{aligned}$$

By assumptions (2.1.17), (2.1.18), the equality $b = b_1+b_2-a$ and Lemma 2.3 (i) we obtain that

$$\begin{aligned}
S_5 &\in \mathfrak{S}_{\frac{1}{a(l-k-1)},\infty} \cdot \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{b_2},\infty} \cdot \mathfrak{S}_{\frac{1}{ak},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty},\\
S_6 &\in \mathfrak{S}_{\frac{1}{a(l-k-1)+b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{b_2},\infty} \cdot \mathfrak{S}_{\frac{1}{ak},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty},\\
S_7 &\in \mathfrak{S}_{\frac{1}{a(l-k-1)},\infty} \cdot \mathfrak{S}_{\frac{1}{b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{ak+b_2},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty},\\
S_8 &\in \mathfrak{S}_{\frac{1}{a(l-k-1)+b_1},\infty} \cdot \mathfrak{S}_{\frac{1}{ak+b_2},\infty} = \mathfrak{S}_{\frac{1}{al+b},\infty}.
\end{aligned}$$

Hence we conclude that

$$T_{l,k}(\lambda_0) \in \mathfrak{S}_{\frac{1}{al+b},\infty}, \tag{2.1.21}$$

for all $k = 1, 2, \ldots, l-2$. Thus, summarizing (2.1.20) and (2.1.21), we obtain that $T_{l,k}(\lambda_0) \in \mathfrak{S}_{\frac{1}{al+b},\infty}$ for all $k = 0, 1, \ldots, l-1$. Now Lemma 2.2 implies the statement. Similarly with the help of Lemma 2.3 (ii) one can show analogous statement for $\mathfrak{S}_p$-classes. $\square$

Remark 2.7. In the proof of the last lemma we used the algebraic identity for $m \geq 2$ and arbitrary elements a, b and c of a non-commutative algebra

$$a^m - b^m = \big(f_0 + h_0\big) + \big(g_{m-1} + h_{m-1}\big) + \sum_{k=1}^{m-2} \big(e_k + f_k + g_k - h_k\big),$$

where

$$\begin{aligned} e_k =& (a^{m-k-1} - c^{m-k-1})(a-b)(b^k - c^k), \\ f_k =& (a^{m-k-1} - c^{m-k-1})(a-b)c^k, \\ g_k =& c^{m-k-1}(a-b)(b^k - c^k), \\ h_k =& c^{m-k-1}(a-b)c^k. \end{aligned}$$

In our case $a = (H-\lambda)^{-1}$, $b = (K-\lambda)^{-1}$ and $c = (L-\lambda)^{-1}$. In applications to elliptic operators we take for L a self-adjoint elliptic operator with known smoothing properties of its resolvent, while smoothing properties of the resolvents of H and K can be unknown, and they may be weaker, see Section 3.3.

2.2 Quasi boundary triples and their Weyl functions

In this section we introduce the abstract concept of quasi boundary triples and associated Weyl functions useful in extension theory. We provide complete proofs of main statements related to this concept. One can find most of these proofs in [BL07, BL11, BLL12] in a slightly different form. We start with with basic statements and definitions of the key objects, further we derive Krein's formulae, study spectral relations of Birman-Schwinger type and give sufficient conditions for self-adjointness of extensions. All this material is intensively used throughout the further chapters.

2.2.1 Definitions and basic properties

The concept of quasi boundary triples is a generalization of the notion of (ordinary) boundary triples from [Bru76, DM91, GorGor91, Ko75]. Quasi boundary triples are particularly useful when dealing with elliptic boundary value problems from an operator and extension theoretic points of view. Generalized boundary triples from [DHMS06, DM95] are a particular case of quasi boundary triples. In this subsection we provide some general facts on quasi boundary triples.

Definition 2.8. Let A be a closed, densely defined, symmetric operator in a Hilbert space $\big(\mathcal{H}, (\cdot,\cdot)_{\mathcal{H}}\big)$. A triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called a *quasi boundary triple* for A^* if $\big(\mathcal{G}, (\cdot,\cdot)_{\mathcal{G}}\big)$ is a Hilbert space and for some linear operator $T \subset A^*$ with $\overline{T} = A^*$ the following holds:

(i) $\Gamma_0, \Gamma_1 : \operatorname{dom} T \to \mathcal{G}$ are linear mappings, and the mapping $\Gamma := \binom{\Gamma_0}{\Gamma_1}$ has dense range in $\mathcal{G} \times \mathcal{G}$;

(ii) $A_0 := T \upharpoonright \ker \Gamma_0$ is a self-adjoint operator in $\mathcal{H}$;

(iii) for all $f, g \in \operatorname{dom} T$ the *abstract Green's identity*

$$(Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} \tag{2.2.1}$$

holds.

We remark that a quasi boundary triple for A^* exists if and only if the deficiency indices $n_\pm(A) = \dim \ker(A^* \mp i)$ of A coincide. Moreover, if $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^*, then A coincides with $T \upharpoonright \ker \Gamma$ and the operator $A_1 := T \upharpoonright \ker \Gamma_1$ is symmetric in $\mathcal{H}$. We also mention that a quasi boundary triple with the additional property $\operatorname{ran} \Gamma_0 = \mathcal{G}$ is a generalized boundary triple in the sense of [DHMS06, DM95].

The proposition below contains a sufficient condition for a triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ to be a quasi boundary triple. It can be found in [BL07, BL11].

Proposition 2.9. *Let $\mathcal{H}$ and $\mathcal{G}$ be Hilbert spaces and let T be a linear operator in $\mathcal{H}$. Assume that $\Gamma_0, \Gamma_1 \colon \operatorname{dom} T \to \mathcal{G}$ are linear mappings such that the following conditions are satisfied:*

(a) $\Gamma = \binom{\Gamma_0}{\Gamma_1} \colon \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ *has dense range, and* $\ker \Gamma$ *is dense in* $\mathcal{H}$*;*

(b) *The identity* (2.2.1) *holds for all* $f, g \in \operatorname{dom} T$*;*

(c) $T \upharpoonright \ker \Gamma_0$ *contains a self-adjoint operator* A_0.

Then $A := T \upharpoonright \ker \Gamma$ *is a closed, densely defined, symmetric operator; the operator* A_0 *coincides with* $T \upharpoonright \ker \Gamma_0$*; the operator* T *is closable and* $\overline{T} = A^*$ *holds. Finally, the triple* $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *is a quasi boundary triple for* A^*.

Proof. As the first preliminary step of the proof we verify that $T^* \subset T$. By the abstract Green's identity the operator $T \upharpoonright \ker \Gamma_0$ is symmetric. Since the symmetric operator $T \upharpoonright \ker \Gamma_0$ contains the self-adjoint operator A_0, these operators coincide, and we have the following chain of inclusions

$$T^* \subset A_0^* = A_0 \subset T. \tag{2.2.2}$$

The abstract Green's identity yields that A is symmetric. Let us show that $A = T^*$. We start with the inclusion

$$A \subset T^*.$$

Let us take an arbitrary $g \in \operatorname{dom} A$ and an arbitrary $f \in \operatorname{dom} T$. Since $g \in \operatorname{dom} A$, we have $\Gamma g = 0$. Thus we get

$$(Tf, g)_{\mathcal{H}} - (f, Ag)_{\mathcal{H}} = (Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} = 0.$$

This calculation implies that $g \in \operatorname{dom} T^*$ and that $T^* g = Ag$. Therefore the inclusion $A \subset T^*$ holds. Next we are aiming to show the opposite inclusion

$$T^* \subset A.$$

Let us now take an arbitrary $g \in \operatorname{dom} T^*$ and an arbitrary $f \in \operatorname{dom} T$. Using the inclusion $T^* \subset T$, which is shown in (2.2.2), we get

$$0 = (Tf, g)_{\mathcal{H}} - (f, T^* g)_{\mathcal{H}} = (Tf, g)_{\mathcal{H}} - (f, Tg)_{\mathcal{H}} = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} + (\Gamma_0 f, -\Gamma_1 g)_{\mathcal{G}}.$$

This means that $\left(\begin{smallmatrix} -\Gamma_1 g \\ \Gamma_0 g \end{smallmatrix}\right)$ is orthogonal to the range of the mapping Γ in the Hilbert space $\mathcal{G} \times \mathcal{G}$. By assumption (a) of the proposition the range of Γ is dense in $\mathcal{G} \times \mathcal{G}$, which implies that $\Gamma g = 0$. We have shown that $g \in \operatorname{dom} A$ and that $T^* g = Tg = Ag$, thus $T^* \subset A$. Altogether this yields that $A = T^*$. Employing, then, the density of $\ker \Gamma$ in $\mathcal{H}$ we obtain that T is closable and that $\overline{T} = A^*$. Now by Definition 2.8 the triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^*. $\square$

Next we recall the definition of the γ-field and the Weyl function associated with the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for A^*. Note that the decomposition

$$\operatorname{dom} T = \operatorname{dom} A_0 \dotplus \ker(T - \lambda) = \ker \Gamma_0 \dotplus \ker(T - \lambda)$$

holds for all $\lambda \in \rho(A_0)$, so that $\Gamma_0 \upharpoonright \ker(T - \lambda)$ is invertible for all $\lambda \in \rho(A_0)$.

Definition 2.10. Let A be a closed, densely defined, symmetric operator in a Hilbert space $\mathcal{H}$. Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for A^* with $T \subset A^*$ and $A_0 = T \upharpoonright \ker \Gamma_0$. Then the (operator-valued) functions γ and M defined by

$$\gamma(\lambda) := \big(\Gamma_0 \upharpoonright \ker(T - \lambda)\big)^{-1} \text{ and } M(\lambda) := \Gamma_1 \gamma(\lambda), \quad \lambda \in \rho(A_0),$$

are called the γ-*field* and the *Weyl function* corresponding to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$.

These definitions coincide with the definitions of the γ-field and the Weyl function in the case that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is an ordinary boundary triple, see [DM91]. Note that for each $\lambda \in \rho(A_0)$ the operator $\gamma(\lambda)$ maps $\operatorname{ran} \Gamma_0$ into $\mathcal{H}$ and $M(\lambda)$ maps $\operatorname{ran} \Gamma_0$ into $\operatorname{ran} \Gamma_1$. Furthermore, as an immediate consequence of the definition of $M(\lambda)$ we obtain that

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda, \qquad f_\lambda \in \ker(T - \lambda), \quad \lambda \in \rho(A_0). \tag{2.2.3}$$

In the next proposition we collect some properties of the γ-field and the Weyl function; all the statements are proven in [BL07], but for completeness of the thesis we provide these proofs. Recall that the space of bounded everywhere defined linear operators from $\mathcal{H}$ into $\mathcal{G}$ is denoted by $\mathcal{B}(\mathcal{H}, \mathcal{G})$. We set $\mathcal{B}(\mathcal{G}) := \mathcal{B}(\mathcal{G}, \mathcal{G})$.

Proposition 2.11. *Let A be a closed, densely defined, symmetric operator in a Hilbert space $\mathcal{H}$. Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for A^* with the γ-field γ and the Weyl function M. Then for $\lambda, \mu \in \rho(A_0)$ the following assertions hold.*

(i) $\gamma(\lambda)$ *is a bounded, densely defined operator from $\mathcal{G}$ into $\mathcal{H}$. The adjoint of $\gamma(\overline{\lambda})$ has the representation*

$$\gamma(\overline{\lambda})^* = \Gamma_1 (A_0 - \lambda)^{-1} \in \mathcal{B}(\mathcal{H}, \mathcal{G}).$$

(ii) *$M(\lambda)$ is a densely defined (in general unbounded) operator in $\mathcal{G}$ and for $\lambda \in \rho(A_0)$ the inclusion $M(\lambda) \subset M(\overline{\lambda})^*$ holds, and*

$$\big(M(\lambda) - M(\overline{\mu})\big)\varphi = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)\varphi, \quad \varphi \in \operatorname{ran}\Gamma_0. \tag{2.2.4}$$

In particular, if $\operatorname{ran}\Gamma_0 = \mathcal{G}$, *then* $M(\lambda) = M(\overline{\lambda})^*$ *and* $M(\lambda) \in \mathcal{B}(\mathcal{G})$.

(iii) *If $A_1 = T \upharpoonright \ker\Gamma_1$ is a self-adjoint operator in $\mathcal{H}$ and $\lambda \in \rho(A_0) \cap \rho(A_1)$, then $M(\lambda)$ maps* $\operatorname{ran}\Gamma_0$ *bijectively onto* $\operatorname{ran}\Gamma_1$, *and*

$$M(\lambda)^{-1}\gamma(\overline{\lambda})^* \in \mathcal{B}(\mathcal{H}, \mathcal{G}).$$

Proof. (i) Let us fix $\lambda \in \rho(A_0)$. Since $\operatorname{dom}\gamma(\lambda) = \operatorname{ran}\Gamma_0$ and the set $\operatorname{ran}\Gamma_0$ is dense in $\mathcal{G}$, the operator $\gamma(\lambda)$ is densely defined. Let us take arbitrary elements $\varphi \in \operatorname{ran}\Gamma_0$ and $g \in \mathcal{H}$. Since $\lambda \in \rho(A_0)$, there exists $h \in \operatorname{dom} A_0$ such that $(A_0 - \lambda)h = g$. Further, applying the abstract Green's identity we get

$$\begin{aligned}\big(\gamma(\overline{\lambda})\varphi, g\big)_{\mathcal{H}} =& \big(\gamma(\overline{\lambda})\varphi, (A_0 - \lambda)h\big)_{\mathcal{H}} = \big(\gamma(\overline{\lambda})\varphi, Th\big)_{\mathcal{H}} - \big(T\gamma(\overline{\lambda})\varphi, h\big)_{\mathcal{H}} = \\ =& \big(\Gamma_0\gamma(\overline{\lambda})\varphi, \Gamma_1 h\big)_{\mathcal{G}} - \big(\Gamma_1\gamma(\overline{\lambda})\varphi, \Gamma_0 h\big)_{\mathcal{G}} = \big(\varphi, \Gamma_1(A_0 - \lambda)^{-1}g\big)_{\mathcal{G}},\end{aligned}$$

where we used that $\Gamma_0 h = 0$. Since $\operatorname{ran}\Gamma_0$ is dense in $\mathcal{G}$, we get from the last calculation that $\gamma(\overline{\lambda})^* = \Gamma_1(A_0 - \lambda)^{-1}$. Note that the operator $\gamma(\overline{\lambda})^*$ is closed and everywhere defined in $\mathcal{H}$. Thus $\gamma(\overline{\lambda})^* \in \mathcal{B}(\mathcal{H}, \mathcal{G})$ and $\gamma(\lambda) \subset \gamma(\lambda)^{**}$ is bounded.

(ii) Let us again fix some $\lambda \in \rho(A_0)$. By definition the operator $M(\lambda)$ maps $\operatorname{ran}\Gamma_0$ into $\operatorname{ran}\Gamma_1$. Since $\operatorname{ran}\Gamma_0$ is dense $\mathcal{G}$, the operator $M(\lambda)$ is densely defined. Let us now take arbitrary $f_\lambda \in \ker(T - \lambda)$ and $g_\mu \in \ker(T - \mu)$. Applying the abstract Green identity (2.2.1) and using the property (2.2.3) of the Weyl function M we obtain

$$\begin{aligned}(\lambda - \overline{\mu})(f_\lambda, g_\mu)_{\mathcal{H}} =& (Tf_\lambda, g_\mu)_{\mathcal{H}} - (f_\lambda, Tg_\mu)_{\mathcal{H}} \\ =& (\Gamma_1 f_\lambda, \Gamma_0 g_\mu)_{\mathcal{G}} - (\Gamma_0 f_\lambda, \Gamma_1 g_\mu)_{\mathcal{G}} \\ =& \big(M(\lambda)\Gamma_0 f_\lambda, \Gamma_0 g_\mu\big)_{\mathcal{G}} - \big(\Gamma_0 f_\lambda, M(\mu)\Gamma_0 g_\mu\big)_{\mathcal{G}}.\end{aligned} \tag{2.2.5}$$

This calculation with $\mu = \overline{\lambda}$ implies that $M(\lambda) \subset M(\overline{\lambda})^*$. Within the notation $\varphi := \Gamma_0 f_\lambda$ and $\psi := \Gamma_0 g_\mu$ we can rewrite the formula (2.2.5) as

$$(\lambda - \overline{\mu})(\gamma(\lambda)\varphi, \gamma(\mu)\psi)_{\mathcal{H}} = \Big(\big(M(\lambda) - M(\overline{\mu})\big)\varphi, \psi\Big)_{\mathcal{G}}$$

Since $\operatorname{dom}(\gamma(\mu)^*) = \mathcal{H}$ and $\operatorname{ran}\Gamma_0$ is dense in $\mathcal{G}$, we get the identity (2.2.4). If $\operatorname{ran}\Gamma_0 = \mathcal{G}$, then $M(\lambda)$ is everywhere defined. Thus $M(\lambda) = M(\overline{\lambda})^*$, $M(\lambda)$ is closed, and hence $M(\lambda) \in \mathcal{B}(\mathcal{G})$.

(iii) The first assertion of this item follows from the decomposition

$$\operatorname{dom} T = \operatorname{dom} A_1 \dot{+} \ker(T - \lambda)$$

which is valid for all $\lambda \in \rho(A_1)$. Indeed, let us fix $\lambda \in \rho(A_1) \cap \rho(A_0)$ and take an arbitrary $\varphi \in \operatorname{ran}\Gamma_1$. Then there exists $f \in \operatorname{dom} T$ such that $\Gamma_1 f = \varphi$. We can decompose f as $f = f_1 + f_\lambda$, where $f_1 \in \operatorname{dom} A_1$ and $f_\lambda \in \ker(T - \lambda)$. Note that by definition of the Weyl function we get

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda = \Gamma_1(f - f_1) = \Gamma_1 f = \varphi,$$

and we conclude that $\varphi \in \operatorname{ran}(M(\lambda))$.

For the second part of (iii) note that $\{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ is also a quasi boundary triple if A_1 is self-adjoint. It is easy to see that in this case the corresponding γ-field is $\widetilde{\gamma}(\lambda) = \gamma(\lambda)M(\lambda)^{-1}$. Since $\operatorname{ran}(\gamma(\overline{\lambda})^*) \subset \operatorname{ran}\Gamma_1$ by item (i), the operator $M(\lambda)^{-1}\gamma(\overline{\lambda})^*$ is defined on $\mathcal{H}$. Now the boundedness of $\widetilde{\gamma}(\lambda)$, which follows from (i), and the relation $M(\lambda) \subset M(\overline{\lambda})^*$ imply that $M(\lambda)^{-1}\gamma(\overline{\lambda})^*$ is bounded. $\square$

Throughout this thesis we shall often use product rules for holomorphic operator-valued functions. Let $\mathcal{H}_i$, $i = 1, \dots, 4$, be Hilbert spaces, U a domain in $\mathbb{C}$ and let $A\colon U \to \mathcal{B}(\mathcal{H}_3, \mathcal{H}_4)$, $B\colon U \to \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3)$, $C\colon U \to \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ be holomorphic operator-valued functions. Then

$$\frac{d^m}{d\lambda^m}\big(A(\lambda)B(\lambda)\big) = \sum_{\substack{p+q=m \\ p,q\geq 0}} \binom{m}{p} A^{(p)}(\lambda)B^{(q)}(\lambda), \tag{2.2.6}$$

$$\frac{d^m}{d\lambda^m}\big(A(\lambda)B(\lambda)C(\lambda)\big) = \sum_{\substack{p+q+r=m \\ p,q,r\geq 0}} \frac{m!}{p!\,q!\,r!} A^{(p)}(\lambda)B^{(q)}(\lambda)C^{(r)}(\lambda) \tag{2.2.7}$$

for $\lambda \in U$. If $A(\lambda)^{-1}$ is invertible for every $\lambda \in U$, then relation (2.2.6) implies the following formula for the derivative of the inverse,

$$\frac{d}{d\lambda}\big(A(\lambda)^{-1}\big) = -A(\lambda)^{-1}A'(\lambda)A(\lambda)^{-1}. \tag{2.2.8}$$

In the next lemma we consider higher derivatives of γ-field and Weyl function associated with some quasi boundary triple.

Lemma 2.12. *For all $\lambda \in \rho(A_0)$ and all $k \in \mathbb{N}$ the following hold.*

(i) $\dfrac{d^k}{d\lambda^k}\gamma(\overline{\lambda})^* = k!\,\gamma(\overline{\lambda})^*(A_0-\lambda)^{-k}$;

(ii) $\dfrac{d^k}{d\lambda^k}\overline{\gamma(\lambda)} = k!(A_0-\lambda)^{-k}\overline{\gamma(\lambda)}$;

(iii) $\overline{\dfrac{d^k}{d\lambda^k}M(\lambda)} = \dfrac{d^{k-1}}{d\lambda^{k-1}}\big(\gamma(\overline{\lambda})^*\overline{\gamma(\lambda)}\,\big) = k!\,\gamma(\overline{\lambda})^*(A_0-\lambda)^{-(k-1)}\overline{\gamma(\lambda)}$.

Proof. (i) We prove the statement by induction. For $k=1$ we have

$$
\begin{aligned}
\frac{d}{d\lambda}\gamma(\overline{\lambda})^* &= \lim_{\mu\to\lambda}\frac{1}{\mu-\lambda}\big(\gamma(\overline{\mu})^* - \gamma(\overline{\lambda})^*\big)\\
&= \lim_{\mu\to\lambda}\frac{1}{\mu-\lambda}\Gamma_1\big((A_0-\mu)^{-1}-(A_0-\lambda)^{-1}\big)\\
&= \lim_{\mu\to\lambda}\Gamma_1(A_0-\mu)^{-1}(A_0-\lambda)^{-1} = \lim_{\mu\to\lambda}\gamma(\overline{\mu})^*(A_0-\lambda)^{-1}\\
&= \gamma(\overline{\lambda})^*(A_0-\lambda)^{-1},
\end{aligned}
$$

where we used Proposition 2.11 (i). If we assume that the statement is true for $k\in\mathbb{N}$, then

$$
\begin{aligned}
\frac{d^{k+1}}{d\lambda^{k+1}}\gamma(\overline{\lambda})^* &= k!\frac{d}{d\lambda}\Big(\gamma(\overline{\lambda})^*(A_0-\lambda)^{-k}\Big)\\
&= k!\left[\Big(\frac{d}{d\lambda}\gamma(\overline{\lambda})^*\Big)(A_0-\lambda)^{-k} + \gamma(\overline{\lambda})^*\frac{d}{d\lambda}(A_0-\lambda)^{-k}\right]\\
&= k!\left[\gamma(\overline{\lambda})^*(A_0-\lambda)^{-1}(A_0-\lambda)^{-k} + \gamma(\overline{\lambda})^* k(A_0-\lambda)^{-k-1}\right]\\
&= k!(1+k)\gamma(\overline{\lambda})^*(A_0-\lambda)^{-(k+1)},
\end{aligned}
$$

which proves the statement in (i) by induction.

(ii) This assertion is obtained from (i) by taking adjoints.

(iii) It follows from Proposition 2.11 (ii) that, for $\varphi \in \operatorname{dom} M(\lambda) = \operatorname{ran}\Gamma_0$,

$$
\frac{d}{d\lambda}M(\lambda)\varphi = \lim_{\mu\to\lambda}\frac{1}{\mu-\lambda}\big(M(\mu)-M(\lambda)\big)\varphi = \lim_{\mu\to\lambda}\gamma(\overline{\lambda})^*\gamma(\mu)\varphi = \gamma(\overline{\lambda})^*\gamma(\lambda)\varphi.
$$

By taking closures we obtain the claim for $k=1$. For $k \geq 2$ we use (2.2.6) to get

$$\overline{\frac{d^k}{d\lambda^k} M(\lambda)} = \frac{d^{k-1}}{d\lambda^{k-1}}\Big(\gamma(\overline{\lambda})^* \overline{\gamma(\lambda)}\Big) = \sum_{\substack{p+q=k-1\\ p,q\geq 0}} \binom{k-1}{p} \Big(\frac{d^p}{d\lambda^p}\gamma(\overline{\lambda})^*\Big) \frac{d^q}{d\lambda^q}\overline{\gamma(\lambda)}$$

$$= \sum_{\substack{p+q=k-1\\ p,q\geq 0}} \binom{k-1}{p} p!\, \gamma(\overline{\lambda})^* (A_0-\lambda)^{-p} q!\, (A_0-\lambda)^{-q}\, \overline{\gamma(\lambda)}$$

$$= \sum_{\substack{p+q=k-1\\ p,q\geq 0}} (k-1)! \gamma(\overline{\lambda})^* (A_0-\lambda)^{-(k-1)} \overline{\gamma(\lambda)} = k! \gamma(\overline{\lambda})^* (A_0-\lambda)^{-(k-1)} \overline{\gamma(\lambda)},$$

which finishes the proof. □

2.2.2 Self-adjointness and Krein's formulae

Throughout this subsection we assume that the following hypothesis holds.

Hypothesis 2.1. *We assume that A is a closed, densely defined, symmetric operator in a Hilbert space $\mathcal{H}$, and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^* with $T \subset A^*$, $A_i = T \upharpoonright \ker \Gamma_i$, $i = 0, 1$, γ-field γ and Weyl function M.*

In the next theorem we show a connection between the point spectra of the operator A_1 and of the operator-valued function $M(\cdot)$, and we provide a factorization for the resolvent difference of A_0 and A_1.

Theorem 2.13. *Assume that Hypothesis 2.1 holds and that the operator A_1 is self-adjoint. Then the following statements hold.*

(i) *For all $\lambda \in \mathbb{R} \cap \rho(A_0)$*

$$\lambda \in \sigma_{\mathrm{p}}(A_1) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}(M(\lambda))$$

and the multiplicities of these eigenvalues coincide.

(ii) *The formula*

$$(A_0-\lambda)^{-1} - (A_1-\lambda)^{-1} = \gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* \tag{2.2.9}$$

holds for all $\lambda \in \rho(A_1) \cap \rho(A_0)$.

Proof. (i) For the proof it is sufficient to show that $\gamma(\lambda)$ maps $\ker M(\lambda)$ onto $\ker(A_1 - \lambda)$ bijectively. For this purpose, let us take an arbitrary $\varphi \in \ker M(\lambda)$. Note that $\gamma(\lambda)\varphi \in \ker(T-\lambda)$ and that

$$\Gamma_1\gamma(\lambda)\varphi = M(\lambda)\varphi = 0.$$

Thus $\gamma(\lambda)\varphi \in \ker(A_1-\lambda)$ and, therefore, $\gamma(\lambda)$ maps $\ker M(\lambda)$ into $\ker(A_1 - \lambda)$. Let us now take an arbitrary $f_\lambda \in \ker(A_1-\lambda)$. By the computation

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda = 0$$

we get that $\Gamma_0 f_\lambda \in \ker M(\lambda)$. Since $\gamma(\lambda)\Gamma_0 f_\lambda = f_\lambda$, we conclude that $\gamma(\lambda)$ maps $\ker M(\lambda)$ onto $\ker(A_1-\lambda)$ surjectively, whereas injectivitity of this mapping follows from its invertibility.

(ii) Let us fix $\lambda \in \rho(A_1)\cap\rho(A_0)$. By item (i) the operator $M(\lambda)$ is invertible. By Proposition 2.11 (iii) $\operatorname{dom}\big(M(\lambda)^{-1}\big) = \operatorname{ran}\Gamma_1$ and by item (i) of the same proposition $\operatorname{ran}\gamma(\overline{\lambda})^* \subset \operatorname{ran}\Gamma_1$. Thus the operator $\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*$ is everywhere defined in $\mathcal{H}$. For an arbitrary element $g \in \mathcal{H}$ we define

$$f := (A_0-\lambda)^{-1}g - \gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g \in \operatorname{dom} T. \tag{2.2.10}$$

By the calculation

$$\begin{aligned}\Gamma_1 f = \Gamma_1(A_0-\lambda)^{-1}g - \Gamma_1\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g = \\ = \gamma(\overline{\lambda})^*g - M(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g = 0\end{aligned}$$

we get that $f \in \operatorname{dom} A_1$. Observe that

$$(A_1-\lambda)f = (T-\lambda)(A_0-\lambda)^{-1}g - (T-\lambda)\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g = g,$$

which implies $f = (A_1-\lambda)^{-1}g$. Recall that g is an arbitrary element of $\mathcal{H}$ and the formula (2.2.9) follows from (2.2.10). ☐

Further we deal with extensions of A, which are restrictions of T corresponding to some abstract boundary condition. Usually [BL07, DM91, DM95] restrictions of T and simultaneously extensions of A are defined for a linear relation $\Theta \subset \mathcal{G}\times\mathcal{G}$ as follows

$$A_\Theta f := Tf, \quad \operatorname{dom} A_\Theta := \Big\{f \in \operatorname{dom} T\colon \Gamma f \in \Theta\Big\}. \tag{2.2.11}$$

For our purposes it turns out to be more convenient to define for a linear operator B in $\mathcal{G}$ the restriction $A_{[B]}$ of T

$$A_{[B]} := Tf, \quad \operatorname{dom} A_{[B]} := \Big\{f \in \operatorname{dom} T\colon B\Gamma_1 f = \Gamma_0 f\Big\}. \tag{2.2.12}$$

Comparing with definition (2.2.11) the operator $A_{[B]}$ corresponds to the linear relation $\Theta = B^{-1}$. For the relation between the operator $A_{[B]}$ and other operators considered in this section see Figure 2.1.

$$\begin{array}{ccccccccc}
 & & A_0 & & & & & & \\
 & \rotatebox{45}{$\subset$} & & \rotatebox{-45}{$\subset$} & & & & & \\
A & \subset & A_{[B]} & \subset & T & \subset & \overline{T} & = & A^*. \\
 & \rotatebox{-45}{$\subset$} & & \rotatebox{45}{$\subset$} & & & & & \\
 & & A_1 & & & & & &
\end{array}$$

Figure 2.1: This figure shows how the operator $A_{[B]}$ is related to the other operators introduced in this section.

In the next proposition we provide a connection between the point spectra of the operator $A_{[B]}$ and of the operator-valued function $I - BM(\cdot)$.

Proposition 2.14. *Assume that Hypothesis 2.1 holds. Let B be a bounded self-adjoint operator in $\mathcal{G}$ and let $A_{[B]}$ be the operator corresponding to B via (2.2.12). Then for all $\lambda \in \mathbb{R} \cap \rho(A_0)$*

$$\lambda \in \sigma_{\rm p}(A_{[B]}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\rm p}(I - BM(\lambda))$$

and the multiplicities of these eigenvalues coincide.

Proof. We use similar type arguments as in the proof of Theorem 2.13 (i). We show that $\gamma(\lambda)$ maps $\ker(I - BM(\lambda))$ onto $\ker(A_{[B]} - \lambda)$ bijectively. Note that for any $\varphi \in \ker(I - BM(\lambda))$ we get

$$B\Gamma_1\gamma(\lambda)\varphi = BM(\lambda)\varphi = \varphi = \Gamma_0\gamma(\lambda)\varphi.$$

Thus $\gamma(\lambda)\varphi \in \ker(A_{[B]} - \lambda)$ and, hence, $\gamma(\lambda)$ maps $\ker(I - BM(\lambda)$ into $\ker(A_{[B]} - \lambda)$. Let us take an arbitrary $f_\lambda \in \ker(A_{[B]} - \lambda)$. Note that

$$(I - BM(\lambda)\Gamma_0 f_\lambda = \Gamma_0 f_\lambda - B\Gamma_1 f_\lambda = 0,$$

and hence $\Gamma_0 f_\lambda \in \ker(I - BM(\lambda))$. Since $\gamma(\lambda)\Gamma_0 f_\lambda = f_\lambda$, we get that $\gamma(\lambda)$ maps $\ker(I - BM(\lambda))$ onto $\ker(A_{[B]} - \lambda)$ surjectively. Whereas the injectivity of this mapping follows from its invertibility. $\square$

Theorem 2.15. *Assume that Hypothesis 2.1 holds. Let B be a bounded self-adjoint operator in $\mathcal{G}$ and let $A_{[B]}$ be the operator corresponding to B via (2.2.12). Assume that $\lambda \in \rho(A_0) \setminus \sigma_{\mathrm{p}}(A_{[B]})$ or, equivalently, that* $\ker(I - BM(\lambda)) = \{0\}$. *Then the following assertions are true:*

(i) *$g \in \operatorname{ran}(A_{[B]} - \lambda)$ if and only if $B\gamma(\overline{\lambda})^* g \in \operatorname{ran}(I - BM(\lambda))$;*

(ii) *for all $g \in \operatorname{ran}(A_{[B]} - \lambda)$ we have*

$$(A_{[B]} - \lambda)^{-1} g = (A_0 - \lambda)^{-1} g + \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g. \tag{2.2.13}$$

Proof. Fix some point $\lambda \in \rho(A_0)$, which is not an eigenvalue of $A_{[B]}$. Then, by Proposition 2.14, $\ker(I - BM(\lambda)) = \{0\}$ and the inverses $(A_{[B]} - \lambda)^{-1}$ and $(I - BM(\lambda))^{-1}$ are the operators in $\mathcal{H}$ and $\mathcal{G}$, respectively.

Let us take arbitrary $g \in \operatorname{ran}(A_{[B]} - \lambda)$. We show that $B\gamma(\overline{\lambda})^* g \in \operatorname{ran}(I - BM(\lambda))$ and that the formula (2.2.13) holds. Set

$$f := (A_{[B]} - \lambda)^{-1} g - (A_0 - \lambda)^{-1} g \in \operatorname{dom} T.$$

Note that $f \in \ker(T - \lambda)$ and, in particular, by (2.2.3)

$$M(\lambda)\Gamma_0 f = \Gamma_1 f. \tag{2.2.14}$$

The application of Γ_0 and Γ_1 to f gives us

$$\Gamma_0 f = \Gamma_0 (A_{[B]} - \lambda)^{-1} g \quad \text{and} \quad \Gamma_1 f = \Gamma_1 (A_{[B]} - \lambda)^{-1} g - \gamma(\overline{\lambda})^* g,$$

where we used Proposition 2.11 (i) in the second formula. Continuing computations, we get

$$\begin{aligned} BM(\lambda)\Gamma_0 f = B\Gamma_1 f &= B\Gamma_1 (A_{[B]} - \lambda)^{-1} g - B\gamma(\overline{\lambda})^* g = \\ &= \Gamma_0 (A_{[B]} - \lambda)^{-1} g - B\gamma(\overline{\lambda})^* g = \Gamma_0 f - B\gamma(\overline{\lambda})^* g, \end{aligned}$$

and further

$$\big(I - BM(\lambda)\big)\Gamma_0 f = B\gamma(\overline{\lambda})^* g.$$

Thus, it holds that $B\gamma(\overline{\lambda})^* g \in \operatorname{ran}(I - BM(\lambda))$ and that

$$\Gamma_0 f = \big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g.$$

Applying then $\gamma(\lambda)$ to both hand sides, we obtain

$$f = \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g.$$

Since g is arbitrary element in $\operatorname{ran}(A_{[B]} - \lambda)$, the formula (2.2.2) holds.

Next we show the converse implication in (i). Assume that

$$B\gamma(\overline{\lambda})^* g \in \operatorname{ran}(I - BM(\lambda)).$$

Since $\operatorname{dom}(I - BM(\lambda)) = \operatorname{dom}\gamma(\lambda)$, we conclude that the element

$$f := (A_0 - \lambda)^{-1} g + \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g \in \operatorname{dom} T \tag{2.2.15}$$

is well-defined. Computing, we get

$$\begin{aligned} B\Gamma_1 f &= B\gamma(\overline{\lambda})^* g + BM(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g \\ &= \big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^* g = \Gamma_0 f. \end{aligned}$$

Thus $f \in \operatorname{dom} A_{[B]}$ and, moreover,

$$(A_{[B]} - \lambda) f = (T - \lambda) f = (T - \lambda)(A_0 - \lambda)^{-1} g + 0 = g,$$

where we used formula (2.2.15). Hence, we get that $g \in \operatorname{ran}(A_{[B]} - \lambda)$. $\square$

Corollary 2.16. *Assume that Hypothesis 2.1 holds. Let B be a bounded self-adjoint operator in $\mathcal{G}$ and let $A_{[B]}$ be the operator corresponding to B via (2.2.12). Assume that $A_{[B]}$ is self-adjoint. Then the following formulae*

$$\begin{aligned} (A_{[B]} - \lambda)^{-1} - (A_0 - \lambda)^{-1} &= \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^*, \\ (A_{[B]} - \lambda)^{-1} - (A_0 - \lambda)^{-1} &= \gamma(\lambda) B\big(I - M(\lambda)B\big)^{-1} \gamma(\overline{\lambda})^* \end{aligned} \tag{2.2.16}$$

hold for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_0)$.

Proof. If the operator $A_{[B]}$ is self-adjoint, then for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_0)$ we get that $\operatorname{ran}(A_{[B]} - \lambda) = \mathcal{H}$ and the first formula in (2.2.16) follows directly from the formula in Theorem 2.15 (ii). The second formula in (2.2.16) follows after certain straightforward transformations of the first formula, which we omit. $\square$

In the next theorem we provide a factorization for the resolvent difference of $A_{[B_1]}$ and $A_{[B_2]}$ assuming that $A_{[B_1]}$ and $A_{[B_2]}$ are both self-adjoint.

Theorem 2.17. *Assume that Hypothesis 2.1 holds. Let B_1 and B_2 be bounded self-adjoint operators in $\mathcal{G}$. Let the operators $A_{[B_1]}$ and $A_{[B_2]}$ correspond to B_1 and B_2 via (2.2.12), respectively. Assume that $A_{[B_1]}$ and $A_{[B_2]}$ are self-adjoint. Then the formula*

$$\begin{aligned} &(A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1} = \\ &\qquad \gamma(\lambda)\big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1}\gamma(\overline{\lambda})^* \end{aligned}$$

holds for all $\lambda \in \rho(A_{[B_2]}) \cap \rho(A_{[B_1]}) \cap \rho(A_0)$.

Proof. We take the difference of the first factorization in Corollary 2.16 applied to $A_{[B_2]}$ and A_0 and the second factorization of the same corollary applied to $A_{[B_1]}$ and A_0, and we get the formula

$$\begin{aligned}(A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1} = \\ \gamma(\lambda)\Big(\big(I - B_2 M(\lambda)\big)^{-1} B_2 - B_1\big(I - M(\lambda)B_1\big)^{-1}\Big)\gamma(\overline{\lambda})^*.\end{aligned}$$

The difference in the middle

$$\big(I - B_2 M(\lambda)\big)^{-1} B_2 - B_1\big(I - M(\lambda)B_1\big)^{-1}$$

can be further factorized as

$$\big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1},$$

which implies the statement. □

The next two lemmas play a role in the proofs of sufficient conditions for self-adjointness of $A_{[B]}$.

Lemma 2.18. *Assume that Hypothesis 2.1 holds. Let B be a bounded self-adjoint operator in $\mathcal{G}$, and let $A_{[B]}$ be the operator corresponding to B via (2.2.12). Then the operator $A_{[B]}$ is symmetric.*

Proof. By the abstract Green's identity we have for arbitrary $f, g \in \operatorname{dom} A_{[B]}$

$$\begin{aligned}(A_{[B]}f, g)_{\mathcal{H}} - (f, A_{[B]}g)_{\mathcal{H}} &= (\Gamma_1 f, \Gamma_0 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} = \\ &= (\Gamma_1 f, B\Gamma_1 g)_{\mathcal{G}} - (B\Gamma_1 f, \Gamma_1 g)_{\mathcal{G}} = 0,\end{aligned} \tag{2.2.17}$$

where we used self-adjointness of B. This calculation shows that the operator $A_{[B]}$ is symmetric. □

Lemma 2.19. *Assume that Hypothesis 2.1 holds, that* $\operatorname{ran}\Gamma_0 = \mathcal{G}$ *and that* $M(\lambda) \in \mathfrak{S}_\infty(\mathcal{G})$. *Let B be a bounded self-adjoint operator in $\mathcal{G}$. Then*

$$\big(I - BM(\lambda)\big)^{-1}, \big(I - M(\lambda)B\big)^{-1} \in \mathcal{B}(\mathcal{G})$$

holds for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Proof. Let us fix $\lambda \in \mathbb{C} \setminus \mathbb{R}$, and suppose that there exists a non-trivial element $\varphi \in \ker(I - BM(\lambda))$. Then $\gamma(\lambda)\varphi \in \ker(T - \lambda)$ and

$$B\Gamma_1\gamma(\lambda)\varphi = BM(\lambda)\varphi = \varphi = \Gamma_0\gamma(\lambda)\varphi.$$

Thus $\gamma(\lambda)\varphi$ is an eigenvector of $A_{[B]}$ corresponding to the non-real eigenvalue λ. This is a contradiction with the fact that $A_{[B]}$ is symmetric proven in Lemma 2.18. Hence, $I - BM(\lambda)$ is injective. By the assumptions on the operators $M(\lambda)$ and B we get that $BM(\lambda) \in \mathfrak{S}_\infty(\mathcal{G})$ and thus $I - BM(\lambda)$ is also surjective. We immediately obtain that $(I - BM(\lambda))^{-1} \in \mathcal{B}(\mathcal{G})$. Analogous arguments show that $(I - M(\lambda)B)^{-1} \in \mathcal{B}(\mathcal{G})$. $\square$

In the next theorem we prove that the operator $A_{[B]}$ is self-adjoint under a certain assumption on the Weyl function and the operator B.

Theorem 2.20. *Assume that Hypothesis 2.1 holds, that* $\operatorname{ran}\Gamma_0 = \mathcal{G}$ *and that* $M(\lambda) \in \mathfrak{S}_\infty(\mathcal{G})$ *for all* $\lambda \in \rho(A_0)$*. Let* B *be a bounded self-adjoint operator in* $\mathcal{G}$ *and let* $A_{[B]}$ *be the operator corresponding to* B *via* (2.2.12)*. Then the operator* $A_{[B]}$ *is self-adjoint in the Hilbert space* $\mathcal{H}$*.*

Proof. By Lemma 2.18 the operator $A_{[B]}$ is symmetric, and by Lemma 2.19 the operator $(I - BM(\lambda))^{-1}$ is bounded and everywhere defined in $\mathcal{G}$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. Thus, according to Theorem 2.15 (i), $\operatorname{ran}(A_{[B]} - \lambda) = \mathcal{H}$ for all such λ and therefore the operator $A_{[B]}$ is self-adjoint. $\square$

In the next theorem we show self-adjointness of $A_{[B]}$ under other assumptions on the Weyl function. We also prove that under these assumptions $A_{[B]}$ is lower-semibounded and we estimate the corresponding lower bound.

Theorem 2.21. *Assume that Hypothesis 2.1 holds, that* A_0 *is semi-bounded, that* $\operatorname{ran}\Gamma_0 = \mathcal{G}$ *and that*

$$\big\|M(\lambda)\big\| \to 0 \quad \text{as } \lambda \to -\infty.$$

Let B *be a bounded self-adjoint operator in* $\mathcal{G}$ *and let* $A_{[B]}$ *be the operator corresponding to* B *via* (2.2.12)*. Then the following statements hold.*

(i) *The operator* $A_{[B]}$ *is self-adjoint in the Hilbert space* $\mathcal{H}$*.*

(ii) *There exists* $r \in \mathbb{R}$ *such that* $(-\infty, r) \subset \rho(A_0)$ *and the condition*

$$\|M(\lambda)\| \cdot \|B\| < 1$$

holds for all $\lambda < r$*. For such* $r \in \mathbb{R}$ *the estimate* $A_{[B]} \geq rI_{\mathcal{H}}$ *holds.*

Proof. According to the assumption on the operator A_0 there exists $r' \in \mathbb{R}$ such that $(-\infty, r') \subset \rho(A_0)$, and by the assumption on the Weyl function the exists $r < r'$ such that for all $\lambda < r$ the condition $\|M(\lambda)\| \cdot \|B\| < 1$ holds. In this case we obtain that $\big(I - BM(\lambda)\big)^{-1} \in \mathcal{B}(\mathcal{G})$ for all $\lambda \in (-\infty, r)$. Then by Theorem 2.15 (i) we get that $\operatorname{ran}(A_{[B]} - \lambda) = \mathcal{H}$ for all $\lambda \in (-\infty, r)$. Note that by Lemma 2.18 the operator $A_{[B]}$ is symmetric. Therefore, the operator $A_{[B]}$ is self-adjoint and satisfies $A_{[B]} \geq r I_{\mathcal{H}}$. □

2.3 Sobolev spaces

Throughout this thesis Sobolev spaces will play an important role. We provide some necessary notations and basic properties. For more details the reader is referred to the monographs [AF03, G09, LM68, McL00]. Furthermore, in this section we derive some consequences of Schatten-von Neumann properties of compact embeddings or compact weighted embeddings between Sobolev spaces of distinct orders. More on this the reader can find in [A90, G96, HT03, T78, Si05].

2.3.1 Notations and basic properties

Let $\Omega \subseteq \mathbb{R}^n$ be one of the following open sets.

(i) The whole space $\mathbb{R}^n$, $n \geq 1$.

(ii) The half-space $\mathbb{R}^n_+ := \big\{(x, x')^\top : x \in \mathbb{R}^{n-1}, x' \in \mathbb{R}_+\big\}$, $n \geq 2$, with the boundary $\partial\mathbb{R}^n_+ = \mathbb{R}^{n-1}$.

(iii) A bounded or an unbounded domain of dimension $n \geq 2$ with a compact C^∞-boundary $\partial\Omega$.

By $H^s(\Omega)$ and $H^s(\partial\Omega)$, $s \geq 0$, we denote the standard (L^2-based) Sobolev spaces of order s of functions in Ω and on $\partial\Omega$, respectively. The Sobolev spaces $W^{k,\infty}(\Omega)$ and $W^{1,\infty}(\partial\Omega)$ of L^∞-functions are defined by

$$\begin{aligned} W^{k,\infty}(\Omega) &:= \big\{f \in L^\infty(\Omega) \colon \partial^\alpha f \in L^\infty(\Omega),\ |\alpha| \leq k\big\}, \qquad k \in \mathbb{N}_0, \\ W^{1,\infty}(\partial\Omega) &:= \big\{h \in L^\infty(\partial\Omega) \colon \nabla h \in L^\infty(\partial\Omega; \mathbb{R}^{n-1})\big\}, \end{aligned}$$

where $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n) \in \mathbb{N}_0^n$ is a multi-index, $|\alpha| := \sum_{i=1}^n \alpha_i$. Observe that the following implications hold:

$$\begin{aligned} f \in H^k(\Omega),\ g \in W^{k,\infty}(\Omega) \quad &\Longrightarrow \quad fg \in H^k(\Omega), \qquad k \in \mathbb{N}_0; \\ h \in H^1(\partial\Omega),\ k \in W^{1,\infty}(\partial\Omega) \quad &\Longrightarrow \quad hk \in H^1(\partial\Omega). \end{aligned} \tag{2.3.1}$$

For our studies we also need some non-standard spaces with mixed regularity. We denote by $H^s_{\partial\Omega}(\Omega)$ with $s \geq 0$ the subspace of $L^2(\Omega)$, which consists of functions that belong to H^s in a neighborhood of $\partial\Omega$, i.e.,

$$
\begin{aligned}
H^s_{\partial\Omega}(\Omega) := \Big\{ f \in L^2(\Omega) \colon \exists \text{ domain } \Omega' \subset \Omega \text{ such that} \\
\partial\Omega' \supset \partial\Omega \text{ and } f \upharpoonright \Omega' \in H^s(\Omega') \Big\}.
\end{aligned}
\tag{2.3.2}
$$

For $k \in \mathbb{N}_0$ we denote by $W^{k,\infty}_{\partial\Omega}(\Omega)$ the subspace of $L^\infty(\Omega)$ which consists of functions that belong to $W^{k,\infty}$ in a neighborhood of $\partial\Omega$, i.e.,

$$
\begin{aligned}
W^{k,\infty}_{\partial\Omega}(\Omega) := \Big\{ f \in L^\infty(\Omega) \colon \exists \text{ domain } \Omega' \subset \Omega \text{ such that} \\
\partial\Omega' \supset \partial\Omega \text{ and } f \upharpoonright \Omega' \in W^{k,\infty}(\Omega') \Big\}.
\end{aligned}
\tag{2.3.3}
$$

Observe that for $k \in \mathbb{N}_0$ the implication

$$
f \in H^k_{\partial\Omega}(\Omega),\ g \in W^{k,\infty}_{\partial\Omega}(\Omega) \quad \Longrightarrow \quad fg \in H^k_{\partial\Omega}(\Omega)
\tag{2.3.4}
$$

holds.

2.3.2 Estimates of singular values related to Sobolev spaces

The first lemma of this subsection turns out to be useful for $\mathfrak{S}_{p,\infty}$-estimates of resolvent power differences of elliptic operators in the case of domains with compact boundaries.

Lemma 2.22. *Let Σ be an $(n-1)$-dimensional compact C^∞-smooth manifold without boundary, let $\mathcal{K}$ be a Hilbert space and $B \in \mathcal{B}(\mathcal{K}, H^{r_1}(\Sigma))$ with* $\operatorname{ran} B \subset H^{r_2}(\Sigma)$ *where $r_2 > r_1 \geq 0$. Then B is compact and its singular values s_k satisfy*

$$
s_k(B) = O\big(k^{-\frac{r_2-r_1}{n-1}}\big), \quad k \to \infty.
$$

In particular, $B \in \mathfrak{S}_{\frac{n-1}{r_2-r_1},\infty}(\mathcal{K}, H^{r_1}(\Sigma))$ and $B \in \mathfrak{S}_p(\mathcal{K}, H^{r_1}(\Sigma))$ for $p > \frac{n-1}{r_2-r_1}$.

Proof. Let $\Lambda_{r_1,r_2} := (I - \Delta^\Sigma_{\mathrm{LB}})^{\frac{r_2-r_1}{2}}$, where $\Delta^\Sigma_{\mathrm{LB}}$ denotes the Laplace–Beltrami operator on Σ. The operator Λ_{r_1,r_2} is an isometric isomorphism from $H^{r_2}(\Sigma)$ onto $H^{r_1}(\Sigma)$. From [A90, (5.39) and the text below] we obtain for the asymptotics of the eigenvalues $\lambda_k(I - \Delta^\Sigma_{\mathrm{LB}}) \sim Ck^{\frac{2}{n-1}}$ with some constant C. Hence,

$$
s_k(\Lambda^{-1}_{r_1,r_2}) = O\big(k^{-\frac{r_2-r_1}{n-1}}\big), \quad k \to \infty.
$$

We can write B in the form

$$B = \Lambda_{r_1,r_2}^{-1}(\Lambda_{r_1,r_2}B). \tag{2.3.5}$$

The operator B is closed as an operator from $\mathcal{K}$ into $H^{r_1}(\Sigma)$, hence also closed as an operator from $\mathcal{K}$ into $H^{r_2}(\Sigma)$, which implies that it is bounded from $\mathcal{K}$ into $H^{r_2}(\Sigma)$. Therefore the operator $\Lambda_{r_1,r_2}B$ is bounded from $\mathcal{K}$ into $H^{r_1}(\Sigma)$, and hence the assertions follow from (2.3.5). $\square$

For the next lemma we need some preparatory work. The following condition on a bounded function $\alpha\colon \mathbb{R}^{n-1} \to \mathbb{R}$ with $n \geq 2$ will play a role

$$\mu\left(\left\{x \in \mathbb{R}^{n-1} : |\alpha(x)| \geq \varepsilon\right\}\right) < \infty \quad \text{for all } \varepsilon > 0, \tag{2.3.6}$$

here μ denotes the Lebesgue measure on $\mathbb{R}^{n-1}$. We remark that condition (2.3.6) includes, e.g., the case that α belongs to $L^q(\mathbb{R}^{n-1})$ for some $q \geq 1$, and the case that $\sup_{|x|\geq r} |\alpha(x)| \to 0$ as $r \to \infty$.

Lemma 2.23. *Let $\mathcal{K}$ be a Hilbert space and let $K \in \mathcal{B}(\mathcal{K}, L^2(\mathbb{R}^{n-1}))$ be an operator with $\operatorname{ran} K \subset H^1(\mathbb{R}^{n-1})$. If $\alpha \in L^\infty(\mathbb{R}^{n-1})$ satisfies condition (2.3.6), then $\alpha K \in \mathfrak{S}_\infty(\mathcal{K}, L^2(\mathbb{R}^{n-1}))$.*

Proof. In view of the assumption on α there exists a sequence

$$\Omega_1 \subset \Omega_2 \subset \cdots \subset \Omega_m \subset \ldots$$

of smooth domains of finite measure whose union is all of $\mathbb{R}^{n-1}$ such that for each $m \in \mathbb{N}$ we have

$$\sup_{\mathbb{R}^{n-1}\setminus\Omega_m} |\alpha(x)| < \tfrac{1}{m}.$$

For each $m \in \mathbb{N}$ let χ_m be the characteristic function of the set Ω_m. Denote by P_m the canonical projection from $L^2(\mathbb{R}^{n-1})$ to $L^2(\Omega_m)$ and by J_m the canonical embedding of $L^2(\Omega_m)$ into $L^2(\mathbb{R}^{n-1})$. Then $\operatorname{ran}(P_m\chi_m K) \subset H^1(\Omega_m)$ and, by embedding statements, $P_m\chi_m K : \mathcal{K} \to L^2(\Omega_m)$ is compact; see [EdEv75, Theorem 3.4 and Theorem 4.11] and [EdEv87, Chapter V]. Since αJ_m is bounded, it turns out that $\alpha\chi_m K = \alpha J_m P_m \chi_m K$ is compact. From the assumption (2.3.6) on α it follows easily that the sequence of operators $\alpha\chi_m K$ converges to αK in the operator-norm topology. Thus also αK is compact, which is the assertion of this lemma. $\square$

Remark 2.24. The condition in Lemma 2.23 can be slightly weakened using the optimal prerequisites on a domain Ω which imply compactness of the embedding of $H^1(\Omega)$ into $L^2(\Omega)$; see, e.g., [EdEv87, Chapter VIII]. To avoid too inconvenient and technical assumptions, we restrict ourselves to the condition (2.3.6).

The lemma below is the main ingredient in the proof of Schatten-von Neumann properties for the resolvent power differences of elliptic operators on the half-space.

Lemma 2.25. *Let $\mathcal{K}$ be a Hilbert space and let $K \in \mathcal{B}(\mathcal{K}, L^2(\mathbb{R}^{n-1}))$ be an operator with $\operatorname{ran} K \subset H^s(\mathbb{R}^{n-1})$ with $s > 0$. Let $\alpha \in L^\infty(\mathbb{R}^{n-1})$ be real-valued.*

(i) *If α is compactly supported, or, if $\frac{n-1}{s} > 2$ and $\alpha \in L^{(n-1)/s}(\mathbb{R}^n)$, then*

$$\alpha K \in \mathfrak{S}_{\frac{n-1}{s},\infty}(\mathcal{K}, L^2(\mathbb{R}^{n-1})).$$

(ii) *If $\alpha \in L^p(\mathbb{R}^{n-1})$ with $p \geq 2$ and $p > \frac{n-1}{s}$, then*

$$\alpha K \in \mathfrak{S}_p(\mathcal{K}, L^2(\mathbb{R}^{n-1})).$$

Let us recall that a function f is said to belong to the *weak Lebesgue space* $L^{p,\infty}(\mathbb{R}^{n-1})$ for some $p > 1$, if the condition

$$\sup_{t>0} \big(t^p \mu\big(\{x \in \mathbb{R}^{n-1} : |f(x)| > t\}\big)\big) < \infty$$

is satisfied, where μ again denotes the Lebesgue measure on $\mathbb{R}^{n-1}$. This will play a role in the following proof.

Proof of Lemma 2.25. Note that in the proof we speak about classes of operator ideals and do not indicate Hilbert spaces $\mathcal{K}$ and $L^2(\mathbb{R}^{n-1})$. Let us assume that α has a compact support and that $\Omega \subset \mathbb{R}^{n-1}$ is a bounded, smooth domain with $\Omega \supset \operatorname{supp} \alpha$. Let P be the canonical projection in $L^2(\mathbb{R}^{n-1})$ onto $L^2(\Omega)$, let J be the canonical embedding of $L^2(\Omega)$ into $L^2(\mathbb{R}^{n-1})$, and let $\widetilde{\alpha} := \alpha|_\Omega$. Since $\operatorname{ran}(PK) \subset H^s(\Omega)$ and Ω is a bounded, smooth domain, the embedding operator from $H^s(\Omega)$ into $L^2(\Omega)$ is contained in the class $\mathfrak{S}_{\frac{n-1}{s},\infty}$, see [HT03, Theorem 7.8]. It follows $PK \in \mathfrak{S}_{\frac{n-1}{s},\infty}$ as a mapping from $\mathcal{K}$ into $L^2(\Omega)$. Since $J\widetilde{\alpha}$ is bounded, we obtain $\alpha K = J\widetilde{\alpha} PK \in \mathfrak{S}_{\frac{n-1}{s},\infty}$.

The proofs of the remaining statements make use of the spectral estimates for the operator αD in $L^2(\mathbb{R}^{n-1})$ with

(2.3.7)
$$D = (I - \Delta_{\mathbb{R}^{n-1}})^{-s/2} = g(-i\nabla), \quad g(x) = (1 + |x|^2)^{-s/2},\ x \in \mathbb{R}^{n-1},$$

where the formal notation $g(-i\nabla)$ can be made precise with the help of the Fourier transform. We remark that D, regarded as an operator from $L^2(\mathbb{R}^{n-1})$ into $H^s(\mathbb{R}^{n-1})$ is an isometric isomorphism. The function g belongs to $L^{(n-1)/s,\infty}(\mathbb{R}^{n-1})$. In fact, one easily verifies that the set $\{x \in \mathbb{R}^{n-1} : |g(x)| > t\}$ is contained in the ball of radius $t^{-1/s}$ centered at zero, and the formula for the volume of a ball leads to the claim. Since $\frac{n-1}{s} > 2$ and $\alpha \in L^{(n-1)/s}(\mathbb{R}^n)$, the result by Cwikel in [Cw77] yields that

$$\alpha D \in \mathfrak{S}_{\frac{n-1}{s},\infty};$$

see also [Si05, Theorem 4.2]. We conclude that

$$\alpha K = \alpha D D^{-1} K \in \mathfrak{S}_{\frac{n-1}{s},\infty}.$$

Thus we have proved (i).

In order to show (ii) let us assume that $\alpha \in L^p(\mathbb{R}^{n-1})$ with $p \geq 2$ and $p > \frac{n-1}{s}$. It is easy to check that g in (2.3.7) belongs to $L^r(\mathbb{R}^{n-1})$ for each $r > \frac{n-1}{s}$. Now we can conclude that α and g are both in $L^p(\mathbb{R}^{n-1})$. Standard result [Si05, Theorem 4.1] implies that

$$\alpha D \in \mathfrak{S}_p.$$

It follows that

$$\alpha K = \alpha D D^{-1} K \in \mathfrak{S}_p.$$

which is the assertion of (ii). $\square$

2.4 Elements of mathematical scattering theory

In this section we define the wave operators and the scattering operator, and discuss some of their basic properties. The study of the wave operators and of the scattering operator was motivated by needs of physics, especially, of quantum mechanics. For a physical point of view we refer to [FM93].

Scattering theory also has its independent mathematical value as a part of perturbation theory of operators, see the monographs [K95, RS79-III, Y92].

Further let $\mathcal{H}$ be a Hilbert space, and let H_0, H be self-adjoint operators acting in $\mathcal{H}$. In the following we denote by P_0^{ac} and P^{ac} the orthogonal projectors onto the absolutely continuous subspaces $\mathcal{H}_0^{(\mathrm{ac})} \subset \mathcal{H}$ and $\mathcal{H}^{(\mathrm{ac})} \subset \mathcal{H}$ of the self-adjoint operators H_0 and H, respectively. The absolutely continuous parts of the operators H and H_0 are specified as

$$H_0^{\mathrm{ac}} := P_0^{\mathrm{ac}} H_0 P_0^{\mathrm{ac}} \quad \text{and} \quad H^{\mathrm{ac}} := P^{\mathrm{ac}} H P^{\mathrm{ac}}.$$

Definition 2.26. The *wave operators* $W_\pm(H, H_0)$ are defined as

$$W_\pm(H_0, H) := s - \lim_{t\to\pm\infty} e^{itH} e^{-itH_0} P_0^{\mathrm{ac}},$$

provided that the corresponding strong limit exists. The wave operators $W_\pm(H_0, H)$ are called *complete*, if

$$\operatorname{ran} W_\pm(H_0, H) = \mathcal{H}_{\mathrm{ac}}(H).$$

Note that $W_\pm(H_0, H)$ are isometric on the absolutely continuous subspace $\mathcal{H}_0^{(\mathrm{ac})}$ of the operator H_0 and satisfy the intertwining property

$$W_\pm(H_0, H) H_0 f = H W_\pm(H_0, H) f \quad \text{for all} \quad f \in \mathcal{H}_0^{(\mathrm{ac})}.$$

Provided that the wave operators for the pair $\{H_0, H\}$ exist and are complete, the absolutely continuous parts H_0^{ac} and H^{ac} are unitarily equivalent. In the thesis we use Birman-Kato criterion for the existence and completeness of the wave operators.

Theorem 2.27 (Birman-Kato)**.** *If for two self-adjoint operators H_0 and H in a Hilbert space $\mathcal{H}$, some $m \in \mathbb{N}$ and an arbitrary $\lambda_0 \in \rho(H_0) \cap \rho(H)$ the resolvent power difference satisfies*

$$(H - \lambda_0)^{-m} - (H_0 - \lambda)^{-m} \in \mathfrak{S}_1(\mathcal{H}),$$

then the corresponding wave operators $W_\pm(H_0, H)$ exist and are complete.

A typical application of the Birman-Kato criterion is the proof of the existence and completeness of the wave operators for a pair of Schrödinger operators

$$H_0 := -\Delta + V_0 \quad \text{and} \quad H = -\Delta + V_0 + V, \tag{2.4.1}$$

acting in the Hilbert space $L^2(\mathbb{R}^n)$. Under the assumption that real-valued potentials V_0 and V satisfy

$$V_0 \in L^\infty(\mathbb{R}^n) \quad \text{and} \quad V(x) \leq \frac{C}{(1+|x|)^\rho}$$

with some constants $C > 0$ and $\rho > n$ the wave operators for the pair $\{H_0, H\}$ exist and are complete. For the proof of the Birman-Kato result, further applications to Schrödinger operators and other criteria for existence and completeness of wave operators the reader is addressed to the monographs [RS79-III, Y92]. It worth mentioning that some other criteria lead to better results for particular classes of operators.

In applications the scattering operator plays an important role, see [Y10].

Definition 2.28. The *scattering operator* S is defined as

$$S(H_0, H) := W_+(H_0, H)^* W_-(H_0, H),$$

provided that the wave operators $W_\pm(H_0, H)$ from Definition 2.26 exist.

If the wave operators are complete, then the scattering operator $S(H_0, H)$ is unitary in $\mathcal{H}_0^{(\mathrm{ac})}$ and it commutes with H_0 in the sense

$$H_0 S(H_0, H) f = S(H_0, H) H_0 f \quad \text{for all } f \in \mathcal{H}_0^{(\mathrm{ac})}.$$

In Chapter 3 we prove in Corollaries 3.14 and 3.16 existence and completeness of the wave operators for pairs of self-adjoint elliptic operators on an exterior domain subject to one elliptic differential expression and with distinct boundary conditions. In Chapter 4 we prove in Corollaries 4.23 and 4.27 existence and completeness of the wave operators for pairs of Schrödinger operators with a δ or δ'-interaction on a hypersurface and of the free Schrödinger operators without singular perturbations. Finally, in Chapter 5 we prove in Corollaries 5.16 and 5.18 existence and completeness of the wave operators for pairs of self-adjoint Robin Laplacians on the half-space. All these proofs use Schatten-von Neumann estimates of resolvent power differences and the Birman-Kato criterion. Our results cover all space dimensions, although in some cases for higher dimensions we assume more smoothness of the coefficients in the differential expressions or in the boundary conditions.

Chapter 3

Elliptic operators on domains with compact boundaries

In this chapter we define self-adjoint realizations of a formally symmetric elliptic partial differential expression subject to Robin and more general non-local self-adjoint boundary conditions on bounded interior and unbounded exterior domains. We provide a modification of the Birman-Schwinger principle for the characterization of the point spectra of these realizations and we prove Krein's formulae for their resolvent differences.

As the underlying problem of this chapter we study Schatten-von Neumann properties of the resolvent power differences of self-adjoint elliptic operators. This problem has a long history in analysis, see Section 3.4 for historical remarks. Our results in this direction extend and complement the works [B62, BS79, BS80, G84, G84a, G11, G11a, M10]. In particular, a new case is presented, where the singular values converge slightly faster than for the well-studied case of the resolvent power difference of Dirichlet and Neumann realizations. From these estimates we come to the conclusions about the existence and completeness of the wave operators. Furthermore, for trace class resolvent power differences we provide formulae for their traces. Recently such a type of trace formulae attracted attention [CGNZ12, Ca02, GZ12] in connection with the spectral shift function. Most of the results of this chapter are contained in the works [BLL$^+$10, BLL12, BLL12b] of the author.

3.1 Preliminaries

Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, be a bounded or an unbounded domain with a compact C^∞-boundary $\partial\Omega$. We denote by $(\cdot,\cdot)$ and $(\cdot,\cdot)_{\partial\Omega}$ the inner products in the Hilbert spaces $L^2(\Omega)$ and $L^2(\partial\Omega)$, respectively.

Throughout this chapter we are concerned with the formally symmetric elliptic partial differential expression

$$(\mathcal{L}f)(x) := -\sum_{j,k=1}^{n} \partial_j \big(a_{jk}\partial_k f\big)(x) + a(x)f(x), \quad x \in \Omega, \tag{3.1.1}$$

with bounded, real-valued coefficients $a_{jk} \in C^\infty(\overline{\Omega})$ satisfying $a_{jk}(x) = a_{kj}(x)$ for all $x \in \overline{\Omega}$ and $j,k = 1,\dots,n$, and a bounded, real-valued coefficient $a \in C^\infty(\overline{\Omega})$. We assume that all the first partial derivatives of the coefficients a_{jk} are bounded. Furthermore, $\mathcal{L}$ is assumed to be uniformly elliptic, i.e. the condition

$$\sum_{j,k=1}^{n} a_{jk}(x)\xi_j\xi_k \geq C\sum_{k=1}^{n} \xi_k^2$$

holds for some $C > 0$, all $\xi = (\xi_1,\dots,\xi_n)^\top \in \mathbb{R}^n$ and $x \in \overline{\Omega}$.

For a function $f \in C^\infty(\overline{\Omega})$ we introduce the following trace

$$\partial_{\mathcal{L}} f|_{\partial\Omega} := \sum_{j,k=1}^{n} a_{jk}\nu_j\partial_k f\big|_{\partial\Omega},$$

with the normal vector field $\vec{\nu} = (\nu_1,\nu_2,\dots,\nu_n)$ pointing outwards Ω. For $s > 3/2$ the trace mapping

$$H^s(\Omega) \ni f \mapsto \big\{f|_{\partial\Omega}, \partial_{\mathcal{L}} f|_{\partial\Omega}\big\} \in H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega) \tag{3.1.2}$$

is the continuous extension of the trace mapping defined on C^∞-functions and the mapping in (3.1.2) is surjective onto $H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega)$.

Besides the Sobolev spaces $H^s(\Omega)$ defined in Section 2.3 the spaces

$$H^s_{\mathcal{L}}(\Omega) := \big\{f \in H^s(\Omega) \colon \mathcal{L}f \in L^2(\Omega)\big\}, \quad s \geq 0, \tag{3.1.3}$$

equipped with the scalar product $(\cdot,\cdot)_s + (\mathcal{L}\cdot,\mathcal{L}\cdot)$ and the corresponding norm will be useful.

Observe that for $s \geq 2$ the spaces $H^s_{\mathcal{L}}(\Omega)$ and $H^s(\Omega)$ coincide. We also note that $H^s_{\mathcal{L}}(\Omega)$, $s \in (0,2)$, can be viewed as an interpolation space between $H^2(\Omega)$ an $H^0_{\mathcal{L}}(\Omega)$. The trace mapping can be extended to a continuous mapping

$$H^s_{\mathcal{L}}(\Omega) \ni f \mapsto \bigl\{f|_{\partial\Omega}, \partial_{\mathcal{L}} f|_{\partial\Omega}\bigr\} \in H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega), \quad s \in [0,2), \tag{3.1.4}$$

where each of the mappings

$$\begin{aligned} H^s_{\mathcal{L}}(\Omega) \ni f &\mapsto f|_{\partial\Omega} \in H^{s-1/2}(\partial\Omega), \quad s \in [0,2), \\ H^s_{\mathcal{L}}(\Omega) \ni f &\mapsto \partial_{\mathcal{L}} f|_{\partial\Omega} \in H^{s-3/2}(\partial\Omega), \quad s \in [0,2), \end{aligned}$$

is surjective, see [LM68, Chapter 2, §7.3].

We also recall from [F67, LM68] (see also [BLL12, Theorem 4.2]) that the second Green's identity holds for all $f, g \in H^{3/2}_{\mathcal{L}}(\Omega)$

$$\bigl(\mathcal{L}f, g\bigr) - \bigl(f, \mathcal{L}g\bigr) = \bigl(f|_{\partial\Omega}, \partial_{\mathcal{L}} g|_{\partial\Omega}\bigr)_{\partial\Omega} - \bigl(\partial_{\mathcal{L}} f|_{\partial\Omega}, g|_{\partial\Omega}\bigr)_{\partial\Omega}. \tag{3.1.5}$$

In view of the assumptions on the coefficients in the expression $\mathcal{L}$ the minimal symmetric operator

$$Af := \mathcal{L}f, \quad \operatorname{dom} A := H^2_0(\Omega),$$

is closed and densely defined in the Hilbert space $L^2(\Omega)$, see, e.g., [ADN59, Be65, Br60], cf. [M10, Section 3.1]. The minimal operator A has infinite deficiency indices, and its adjoint operator has the form

$$A^* f = \mathcal{L}f, \quad \operatorname{dom} A^* = \bigl\{f \in L^2(\Omega) \colon \mathcal{L}f \in L^2(\Omega)\bigr\}.$$

The self-adjoint extensions of A subject to Dirichlet and Neumann boundary conditions

$$\begin{aligned} A_{\mathrm{D}} f &:= \mathcal{L}f, \quad \operatorname{dom} A_{\mathrm{D}} := \bigl\{f \in H^2(\Omega) \colon f|_{\partial\Omega} = 0\bigr\}, \\ A_{\mathrm{N}} f &:= \mathcal{L}f, \quad \operatorname{dom} A_{\mathrm{N}} := \bigl\{f \in H^2(\Omega) \colon \partial_{\mathcal{L}} f|_{\partial\Omega} = 0\bigr\}, \end{aligned} \tag{3.1.6}$$

will be important later. For the proofs of the self-adjointness of the operators A_{D} and A_{N} we refer to [Br60, Theorem 5 (iii)] and [Be65, Theorem 7.1 (a)].

3.2 Elliptic operators with general self-adjoint boundary conditions

In this section we use quasi boundary triples for a definition and study of self-adjoint realizations $A_{[B]}$ of $\mathcal{L}$ subject to the non-local boundary condition of the form

$$Bf|_{\partial\Omega} = \partial_{\mathcal{L}} f|_{\partial\Omega}$$

with a bounded self-adjoint operator B in $L^2(\partial\Omega)$.

3.2.1 A quasi boundary triple and its Weyl function

For a proper definition of a quasi boundary triple for A^* we specify the operator T as below

$$Tf := \mathcal{L}f, \quad \operatorname{dom} T := H^{3/2}_{\mathcal{L}}(\Omega), \tag{3.2.1}$$

where the space $H^{3/2}_{\mathcal{L}}(\Omega)$ is defined as in (3.1.3), and we introduce the boundary mappings

$$\begin{aligned} &\Gamma_0 \colon \operatorname{dom} T \to L^2(\partial\Omega), \quad \Gamma_0 f := \partial_{\mathcal{L}} f|_{\partial\Omega},\\ &\Gamma_1 \colon \operatorname{dom} T \to L^2(\partial\Omega), \quad \Gamma_1 f := f|_{\partial\Omega}. \end{aligned} \tag{3.2.2}$$

In the first proposition of this section we prove that the triple $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^* and we show also some basic properties of this quasi boundary triple.

Proposition 3.1. *Let the self-adjoint operators A_{N} and A_{D} be as in (3.1.6). Let the operator T be as in (3.2.1) and the mappings Γ_0, Γ_1 be as in (3.2.2). Then the triple $\Pi = \{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^*. The restrictions of T to the kernels of the boundary mappings are*

$$T \upharpoonright \ker \Gamma_0 = A_{\mathrm{N}} \quad \textit{and} \quad T \upharpoonright \ker \Gamma_1 = A_{\mathrm{D}};$$

and the ranges of these mappings are

$$\operatorname{ran} \Gamma_0 = L^2(\partial\Omega) \quad \textit{and} \quad \operatorname{ran} \Gamma_1 = H^1(\partial\Omega).$$

Proof. In order to show that the triple Π is a quasi boundary triple for A^* we employ Proposition 2.9. Let us check that the triple Π satisfies conditions (a), (b) and (c) of that proposition. Since $H^2(\Omega) \subset \operatorname{dom} T$, by (3.1.2) we have

$$H^{1/2}(\partial\Omega) \times H^{3/2}(\partial\Omega) \subset \operatorname{ran} \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix}.$$

The set $H^{1/2}(\partial\Omega) \times H^{3/2}(\partial\Omega)$ is, clearly, dense in $L^2(\partial\Omega) \times L^2(\partial\Omega)$. Note that the set $\ker \Gamma_0 \cap \ker \Gamma_1 \supset C_0^\infty(\Omega)$ is dense in $L^2(\Omega)$. Therefore the condition (a) is verified. The abstract Green's identity

$$\big(Tf, g\big) - \big(f, Tg\big) = \big(\Gamma_1 f, \Gamma_0 g\big)_{\partial\Omega} - \big(\Gamma_0 f, \Gamma_1 g\big)_{\partial\Omega}$$

for all $f, g \in \operatorname{dom} T$ is equivalent to (3.1.5). That is the condition (b) holds. The operator $T \upharpoonright \ker \Gamma_0$ contains the self-adjoint elliptic operator A_{N} subject to the Neumann boundary condition on $\partial\Omega$. Thus the condition (c) holds for the triple Π, and by Proposition 2.9 the triple Π is a quasi boundary triple for the adjoint of the closed, densely defined, symmetric operator $T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1)$. It remains to show that $T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1) = A$. Indeed, the restriction $T \upharpoonright \ker \Gamma_0$ contains the self-adjoint operator A_{N} and the restriction $T \upharpoonright \ker \Gamma_1$ contains the self-adjoint operator A_{D}. By the abstract Green's identity operators $T \upharpoonright \ker \Gamma_0$ and $T \upharpoonright \ker \Gamma_1$ are both symmetric, thus $T \upharpoonright \ker \Gamma_0 = A_{\mathrm{N}}$ and $T \upharpoonright \ker \Gamma_1 = A_{\mathrm{D}}$. As a consequence of these considerations we get

$$T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1) = (T \upharpoonright \ker \Gamma_0) \cap (T \upharpoonright \ker \Gamma_1) = A_{\mathrm{N}} \cap A_{\mathrm{D}} = A.$$

Hence the triple Π is a quasi boundary triple for A^*.

The properties of the boundary mappings

$$\operatorname{ran} \Gamma_0 = L^2(\partial\Omega) \quad \text{and} \quad \operatorname{ran} \Gamma_1 = H^1(\partial\Omega),$$

follow from (3.1.4). □

In the next proposition we clarify the basic properties of the γ-field and the Weyl function associated with the quasi boundary triple Π from Proposition 3.1. In the terminology of [G96, McL00] these operators turn out to be the *Poisson operator* and the *Neumann-to-Dirichlet map*, respectively.

Proposition 3.2. *Let the self-adjoint operators A_{D} and A_{N} be as in (3.1.6) Let Π be the quasi boundary triple from Proposition 3.1. Let γ and M be the γ-field and the Weyl function associated with the quasi boundary triple Π as in Definition 2.10.*

(i) *The γ-field γ is defined for all $\lambda \in \rho(A_{\mathrm{N}})$ and*

$$\gamma(\lambda)\colon L^2(\partial\Omega) \to L^2(\Omega), \qquad \gamma(\lambda)\varphi := f_\lambda(\varphi),$$

where $f_\lambda(\varphi)$ is the unique solution in the space $H^{3/2}_{\mathcal{L}}(\Omega)$ of the problem

$$\begin{aligned} (\mathcal{L} - \lambda) f &= 0, \quad \text{in } \Omega, \\ \partial_{\mathcal{L}} f|_{\partial\Omega} &= \varphi, \quad \text{on } \partial\Omega. \end{aligned}$$

(ii) *The Weyl function M is defined for all $\lambda \in \rho(A_{\mathrm{N}})$ and*

$$M(\lambda)\colon L^2(\partial\Omega) \to L^2(\partial\Omega), \qquad M(\lambda)\varphi = f_\lambda(\varphi)|_{\partial\Omega},$$

where $f_\lambda(\varphi) = \gamma(\lambda)\varphi$. For all $\lambda \in \rho(A_{\mathrm{N}})$ $\big(\lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}})\big)$ the operator $M(\lambda)$ maps $L^2(\partial\Omega)$ into (onto) $H^1(\partial\Omega)$. The operator $M(\lambda)$ is compact for all $\lambda \in \rho(A_{\mathrm{N}})$.

Proof. (i) The mapping properties of the γ-field γ follow from (3.2.1), (3.2.2) and Definition 2.10.

(ii) The mapping properties of the Weyl function M follow from (3.2.2), Definition 2.10, Proposition 2.11 (iii) and Proposition 3.1. The compactness of the operator $M(\lambda)$ follows from the compactness of the embedding of $H^1(\partial\Omega)$ into $L^2(\partial\Omega)$, cf. Lemma 2.22. □

3.2.2 Self-adjointness and Krein's formulae

In the next theorem we establish a relation between the point spectra of the self-adjoint operator A_{D} and of the operator-valued function $M(\cdot)$. Moreover, we provide a factorization (Krein's formula) for the resolvent difference of A_{N} and A_{D}.

Theorem 3.3. *Let A_{N} and A_{D} be the self-adjoint operators as in* (3.1.6). *Let γ and M be the γ-field and the Weyl function from Proposition 3.2. Then the following statements hold.*

(i) *For all $\lambda \in \mathbb{R} \cap \rho(A_{\mathrm{N}})$*

$$\lambda \in \sigma_{\mathrm{p}}(A_{\mathrm{D}}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}\big(M(\lambda)\big)$$

and the multiplicities of the eigenvalues coincide.

(ii) *The formula*

$$(A_{\mathrm{N}} - \lambda)^{-1} - (A_{\mathrm{D}} - \lambda)^{-1} = \gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^* \tag{3.2.3}$$

holds for all $\lambda \in \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$.

Proof. (i) The equivalence between the point spectra follows from Theorem 2.13 (i) with the self-adjoint operator $A_1 = A_{\mathrm{D}}$.

(ii) Krein's formula follows from Theorem 2.13 (ii) with $A_0 = A_{\mathrm{N}}$ and $A_1 = A_{\mathrm{D}}$. □

As in (2.2.12) we introduce a family of restrictions of T parametrized by an operator acting on the boundary.

Definition 3.4. We define for a bounded self-adjoint operator B in $L^2(\partial\Omega)$ the restriction $A_{[B]}$ of T as below

$$A_{[B]} := T \upharpoonright \ker(B\Gamma_1 - \Gamma_0), \tag{3.2.4}$$

which is equivalent to

$$A_{[B]}f := \mathcal{L}f, \quad \operatorname{dom} A_{[B]} := \Big\{ f \in H^{3/2}_{\mathcal{L}}(\Omega) \colon Bf|_{\partial\Omega} = \partial_{\mathcal{L}} f|_{\partial\Omega} \Big\}.$$

If B is a multiplication operator with a real-valued function $\beta \in L^\infty(\partial\Omega)$, then we write $A_{[\beta]}$ instead of $A_{[B]}$. For the relation between the operator $A_{[B]}$ and the other operators considered in this section see Figure 3.1. In the next theorem we show that $A_{[B]}$ is self-adjoint. We establish a characterization of the point spectrum of $A_{[B]}$ in terms of the point spectrum of the operator-valued function $I - BM(\cdot)$. This characterization can be viewed as an analogue of the Birman-Schwinger principle. Moreover, we provide a factorization (Krein's formula) for the resolvent difference of $A_{[B]}$ and A_{N}.

$$\begin{array}{ccccccccc}
 & & A_{\mathrm{N}} & & & & & & \\
 & \rotatebox{45}{$\subset$} & & \rotatebox{-45}{$\subset$} & & & & & \\
A & \subset & A_{[B]} & \subset & T & \subset & \overline{T} & = & A^*. \\
 & \rotatebox{-45}{$\subset$} & & \rotatebox{45}{$\subset$} & & & & & \\
 & & A_{\mathrm{D}} & & & & & &
\end{array}$$

Figure 3.1: This figure shows how the operator $A_{[B]}$ is related to the other operators introduced in this chapter. The operators A_{N}, A_{D} and $A_{[B]}$ are self-adjoint in $L^2(\Omega)$, cf. Theorem 3.5.

Theorem 3.5. *Let A_{N} be the self-adjoint operator as in (3.1.6). Let γ and M be the γ-field and the Weyl function from Proposition 3.2. Let B be a bounded self-adjoint operator in $L^2(\partial\Omega)$. Let $A_{[B]}$ be the operator corresponding to B via (3.2.4). Then the following statements hold.*

(i) *The operator $A_{[B]}$ is self-adjoint in the Hilbert space $L^2(\Omega)$.*

(ii) *For all* $\lambda \in \rho(A_\mathrm{N}) \cap \mathbb{R}$

$$\lambda \in \sigma_\mathrm{p}(A_{[B]}) \quad \Longleftrightarrow \quad 0 \in \sigma_\mathrm{p}(I - BM(\lambda))$$

and the multiplicities of these eigenvalues coincide.

(iii) *The formulae*

$$(A_{[B]} - \lambda)^{-1} - (A_\mathrm{N} - \lambda)^{-1} = \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^*,$$
$$(A_{[B]} - \lambda)^{-1} - (A_\mathrm{N} - \lambda)^{-1} = \gamma(\lambda)B\big(I - M(\lambda)B\big)^{-1} \gamma(\overline{\lambda})^*$$

hold for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_\mathrm{N})$.

Proof. (i) By Proposition 3.1 the range of the boundary mapping Γ_0 coincides with $L^2(\partial\Omega)$. According to Proposition 3.2 (ii) the values of the Weyl function M are compact operators. By the assumptions the operator B is bounded and self-adjoint in $L^2(\partial\Omega)$ and the statement follows from Theorem 2.20.

(ii) The equivalence between the point spectra follows from Proposition 2.14.

(iii) Krein's formulae follow from self-adjointness of $A_{[B]}$ and Corollary 2.16 with $A_0 = A_\mathrm{N}$. □

In the next theorem we obtain a factorization (Krein's formula) for the resolvent difference of $A_{[B_1]}$ and $A_{[B_2]}$.

Theorem 3.6. *Let* A_N *be the self-adjoint operator in* (3.1.6). *Let* γ *and* M *be the* γ*-field and the Weyl function from Proposition 3.2. Let* B_1 *and* B_2 *be bounded self-adjoint operators in* $L^2(\partial\Omega)$. *Let* $A_{[B_1]}$ *and* $A_{[B_2]}$ *be the self-adjoint operators corresponding via* (3.2.4) *to* B_1 *and* B_2, *respectively. Then the formula*

$$(A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1} =$$
$$\gamma(\lambda)\big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1}\gamma(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{[B_2]}) \cap \rho(A_{[B_1]}) \cap \rho(A_\mathrm{N})$. *In this formula the middle terms on the right-hand side satisfy* $(I - B_2 M(\lambda))^{-1}, (I - M(\lambda)B_1)^{-1} \in \mathcal{B}\big(L^2(\partial\Omega)\big)$.

Proof. Since the operators $A_{[B_1]}$ and $A_{[B_2]}$ are both self-adjoint by Theorem 3.5 (i), Krein's formula follows from Theorem 2.17. The properties of the middle terms are a consequence of Lemma 2.19. □

It follows from Definition 3.4 that $\operatorname{dom} A_{[B]} \subset H^{3/2}(\Omega)$. It is also expected that certain smoothing properties of the operator B in the boundary condition lead to the inclusion $\operatorname{dom} A_{[B]} \subset H^2(\Omega)$. In the next theorem we clarify these smoothing properties. This result is also proved in [G11a, Proposition 2.3 (i)] and [Be65, Theorem 7.1 (a)] by other methods.

Theorem 3.7. *Let B be a bounded self-adjoint operator in $L^2(\partial\Omega)$. Let $A_{[B]}$ be the operator corresponding to B via (3.2.4). Assume that*

$$f \in H^1(\partial\Omega) \quad \Longrightarrow \quad Bf \in H^{1/2}(\partial\Omega).$$

Then the inclusion $\operatorname{dom} A_{[B]} \subset H^2(\Omega)$ *holds.*

Proof. Let f be an arbitrary function from $\operatorname{dom} A_{[B]} \subset \operatorname{dom} T$. Let us fix $\lambda \in \mathbb{C} \setminus \mathbb{R}$. In view of the decomposition

$$\operatorname{dom} T = \operatorname{dom} A_{\mathrm{N}} \dotplus \ker(T - \lambda) \tag{3.2.5}$$

we write f as $f = f_{\mathrm{N}} + f_\lambda$ with $f_{\mathrm{N}} \in \operatorname{dom} A_{\mathrm{N}}$ and $f_\lambda \in \ker(T - \lambda)$. Observe that by (3.1.6) the component $f_{\mathrm{N}} \in H^2(\Omega)$. It remains to show that also $f_\lambda \in H^2(\Omega)$. Indeed, Proposition 3.1 implies that $\Gamma_1 f_\lambda \in H^1(\partial\Omega)$, and the assumption of the theorem yields that

$$\Gamma_0 f_\lambda = B\Gamma_1 f_\lambda \in H^{1/2}(\partial\Omega).$$

In view of the decomposition (3.2.5) and the trace theorem (3.1.2) the mapping Γ_0 is a bijection between the spaces $\ker(T - \lambda) \cap H^2(\Omega)$ and $H^{1/2}(\partial\Omega)$. Thus $\Gamma_0 f_\lambda \in H^{1/2}(\partial\Omega)$ implies that $f_\lambda \in H^2(\Omega)$. Since f_{N} and f_λ both belong to $H^2(\Omega)$, we clearly get that $f \in H^2(\Omega)$ and the claim is proven. $\square$

As a consequence of the last theorem we provide assumptions on the function β for H^2-regularity of the operator domain of $A_{[\beta]}$

Corollary 3.8. *Assume that a real-valued β satisfies $\beta \in W^{1,\infty}(\partial\Omega)$. Then the inclusion* $\operatorname{dom} A_{[\beta]} \subset H^2(\Omega)$ *holds.*

Proof. By (2.3.1) the operator of multiplication with β satisfies the implication

$$f \in H^1(\partial\Omega) \quad \Longrightarrow \quad \beta f \in H^1(\partial\Omega) \subset H^{1/2}(\partial\Omega),$$

and the claim follows from the last theorem. $\square$

3.3 Operator ideal properties of resolvent power differences and trace formulae

The main results of this section are $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power differences of self-adjoint elliptic operators. As a consequence of these estimates we get the existence and completeness of the wave operators for the scattering pairs formed by two self-adjoint elliptic operators on exterior domains. In the case of trace class resolvent power differences we provide trace formulae, where the trace of the resolvent power difference is reduced to the trace of an operator acting on the boundary.

3.3.1 Elliptic regularity and related $\mathfrak{S}_{p,\infty}$-estimates

In this subsection we provide estimates of the singular values of the γ-field and the Weyl function from Proposition 3.2, their derivatives and some related compact operators. For this purpose we use properties of the compact embeddings between Sobolev spaces, given in Lemma 2.22, and elliptic regularity theory.

Furthermore, we make use of the local Sobolev spaces $H^s_{\partial\Omega}(\Omega)$ defined in Subsection 2.3.1. Note that for all $s \geq 0$ and $\lambda \in \rho(A_{\mathrm{N}})$ the implication

$$f \in H^s_{\partial\Omega}(\Omega) \quad \Longrightarrow \quad (A_{\mathrm{N}} - \lambda)^{-1} f \in H^{s+2}_{\partial\Omega}(\Omega) \tag{3.3.1}$$

holds, see [McL00, Theorem 4.18], where this property is formulated in the language of regularity of the solutions for boundary value problems.

In the next lemma we show certain smoothing properties of the γ-field γ and the Weyl function M from Proposition 3.2. This lemma is used in the proof of Theorem 3.12 in the next subsection.

Lemma 3.9. *Let γ and M be the γ-field and the Weyl function from Proposition 3.2. For all $s \geq 0$ the following holds:*

(i) $\operatorname{ran}\big(\gamma(\lambda) \upharpoonright H^s(\partial\Omega)\big) \subset H^{s+\frac{3}{2}}_{\partial\Omega}(\Omega)$ *for all* $\lambda \in \rho(A_{\mathrm{N}})$*;*

(ii) $\operatorname{ran}\big(\gamma(\overline{\lambda})^* \upharpoonright H^s_{\partial\Omega}(\Omega)\big) \subset H^{s+\frac{3}{2}}(\partial\Omega)$ *for all* $\lambda \in \rho(A_{\mathrm{N}})$*;*

(iii) $\operatorname{ran}\big(M(\lambda) \upharpoonright H^s(\partial\Omega)\big) \subset H^{s+1}(\partial\Omega)$ *for all* $\lambda \in \rho(A_{\mathrm{N}})$*;*

(iv) $\operatorname{ran}\big(M(\lambda) \upharpoonright H^s(\partial\Omega)\big) = H^{s+1}(\partial\Omega)$ *for all* $\lambda \in \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$*.*

Proof. It follows from the decomposition $\operatorname{dom} T = \operatorname{dom} A_{\mathrm{N}} \dotplus \ker(T-\lambda)$, $\lambda \in \rho(A_{\mathrm{N}})$, and the properties of the Neumann trace [LM68, Chapter 2, §7.3] that the restriction of the mapping Γ_0 to

$$\ker(T-\lambda) \cap H^{s+\frac{3}{2}}_{\partial\Omega}(\Omega)$$

is a bijection onto $H^s(\partial\Omega)$. Hence, by the definition of the γ-field, we obtain

$$\operatorname{ran}\bigl(\gamma(\lambda) \restriction H^s(\partial\Omega)\bigr) = \ker(T-\lambda) \cap H^{s+\frac{3}{2}}_{\partial\Omega}(\Omega) \subset H^{s+\frac{3}{2}}_{\partial\Omega}(\Omega).$$

Thus the claim (i) is shown.

According to Proposition 2.11 (i) and the definition of Γ_1 we have

$$\gamma(\overline{\lambda})^* = \Gamma_1(A_{\mathrm{N}}-\lambda)^{-1}.$$

The properties of the Dirichlet trace [LM68, Chapter 2, §7.3] and the smoothing property (3.3.1) yield the inclusion

$$\operatorname{ran}\bigl(\gamma(\overline{\lambda})^* \restriction H^s_{\partial\Omega}(\Omega)\bigr) \subset H^{s+\frac{3}{2}}(\partial\Omega)$$

for all $s \geq 0$. Thus we have shown assertion (ii).

Assertion (iii) follows from the definition of $M(\lambda)$, item (i), the fact that Γ_1 is the trace operator and properties of the latter.

To verify (iv) let $\psi \in H^{s+1}(\partial\Omega)$. Since $\lambda \in \rho(A_{\mathrm{D}})$, we have the decomposition $\operatorname{dom} T = \operatorname{dom} A_{\mathrm{D}} \dotplus \ker(T-\lambda)$ and there exists a unique function $f_\lambda \in \ker(T-\lambda) \cap H^{s+\frac{3}{2}}_{\partial\Omega}(\Omega)$ such that $f_\lambda|_{\partial\Omega} = \psi$. Hence

$$\Gamma_0 f_\lambda = \varphi \in H^s(\partial\Omega) \qquad \text{and} \qquad M(\lambda)\varphi = \psi,$$

that is, $H^{s+1}(\partial\Omega) \subset \operatorname{ran}\bigl(M(\lambda) \restriction H^s(\partial\Omega)\bigr)$, and (iii) implies the assertion. □

Another application of the smoothing property (3.3.1) gives the following proposition, in which we provide certain preliminary $\mathfrak{S}_{p,\infty}$-estimates that are useful in the proofs of the main results in the next subsection.

Proposition 3.10. *Let A_{N} be the self-adjoint operator from (3.1.6), and let γ be the γ-field from Proposition 3.2. Then for $\lambda, \mu \in \rho(A_{\mathrm{N}})$ and $k \in \mathbb{N}_0$ the following statements hold:*

(a) $\gamma(\mu)^*(A_{\mathrm{N}}-\lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\bigl(L^2(\Omega), L^2(\partial\Omega)\bigr)$;

(b) $(A_{\mathrm{N}} - \lambda)^{-k}\gamma(\mu) \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\partial\Omega), L^2(\Omega)\big)$;

(c) $\gamma(\mu)^*(A_{\mathrm{N}} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+1/2},\infty}\big(L^2(\Omega), H^1(\partial\Omega)\big)$.

Proof. As $\operatorname{ran}(A_{\mathrm{N}} - \lambda)^{-1} = \operatorname{dom} A_{\mathrm{N}} \subset H^2_{\partial\Omega}(\Omega)$ we conclude from (3.3.1) that the inclusion

$$\operatorname{ran}\Big((A_{\mathrm{N}} - \overline{\mu})^{-1}(A_{\mathrm{N}} - \lambda)^{-k}\Big) \subset H^{2k+2}_{\partial\Omega}(\Omega)$$

holds for all $k \in \mathbb{N}_0$. Moreover, by Proposition 3.1 we have $A_{\mathrm{N}} = T \upharpoonright \ker \Gamma_0$, and Proposition 2.11 (i) implies

$$\gamma(\mu)^*(A_{\mathrm{N}} - \lambda)^{-k} = \Gamma_1(A_{\mathrm{N}} - \overline{\mu})^{-1}(A_{\mathrm{N}} - \lambda)^{-k}$$

and hence

$$\operatorname{ran}\big(\gamma(\mu)^*(A_{\mathrm{N}} - \lambda)^{-k}\big) \subset H^{2k+3/2}(\partial\Omega) \tag{3.3.2}$$

by the properties of the trace map Γ_1, cf. (3.1.2). Now the estimate (a) follows from (3.3.2) and Lemma 2.22 with $\mathcal{K} = L^2(\Omega)$, $\Sigma = \partial\Omega$, $r_1 = 0$ and $r_2 = 2k + \frac{3}{2}$. The estimate (b) follows from the estimate (a) by taking the adjoint. The estimate (c) follows from (3.3.2) and Lemma 2.22 with $\mathcal{K} = L^2(\Omega)$, $\Sigma = \partial\Omega$, $r_1 = 1$ and $r_2 = 2k + \frac{3}{2}$. □

In the proofs of the trace formulae we use estimates of singular values for the derivatives of the γ-field γ and the Weyl function M associated with the quasi boundary triple from Proposition 3.1.

Proposition 3.11. *Let γ and M be the γ-field γ and the Weyl function from Proposition 3.2. Then for all $\lambda \in \rho(A_{\mathrm{N}})$ the following holds:*

(i) *for $k \in \mathbb{N}_0$*

$$\frac{d^k}{d\lambda^k}\gamma(\lambda) \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\partial\Omega), L^2(\Omega)\big),$$
$$\frac{d^k}{d\lambda^k}\gamma(\overline{\lambda})^* \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\Omega), L^2(\partial\Omega)\big);$$

(ii) *for $k \in \mathbb{N}_0$*

$$\frac{d^k}{d\lambda^k}M(\lambda) \in \mathfrak{S}_{\frac{n-1}{2k+1},\infty}\big(L^2(\partial\Omega)\big).$$

Proof. The claim (i) follows from Lemma 2.12 (i), (ii) and Proposition 3.10 (a), (b). By Lemma 2.12 (iii)

$$\frac{d^k}{d\lambda^k}M(\lambda) = k!\,\gamma(\overline{\lambda})^*(A_{\rm N}-\lambda)^{-(k-1)}\gamma(\lambda).$$

Then Proposition 3.10 (a) gives us

$$\frac{d^k}{d\lambda^k}M(\lambda) \in \mathfrak{S}_{\frac{n-1}{2(k-1)+3/2},\infty}\cdot\mathfrak{S}_{\frac{n-1}{3/2},\infty} = \mathfrak{S}_{\frac{n-1}{2k+1},\infty},$$

where the last equality follows from Lemma 2.3 (i). That is the claim (ii). □

3.3.2 Resolvent power differences in $\mathfrak{S}_{p,\infty}$-classes and trace formulae

In the next theorem we prove $\mathfrak{S}_{p,\infty}$-properties for the resolvent power difference of the self-adjoint elliptic operators $A_{\rm D}$ and $A_{\rm N}$. In the case, that the resolvent power difference is in the trace class, we provide the corresponding trace formula.

Theorem 3.12. *Let $A_{\rm D}$ and $A_{\rm N}$ be the self-adjoint operators defined in (3.1.6). Then the following statements hold.*

(i) *For all $\lambda \in \rho(A_{\rm N})\cap\rho(A_{\rm D})$ and all $m\in\mathbb{N}$*

$$(A_{\rm N}-\lambda)^{-m}-(A_{\rm D}-\lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}\big(L^2(\Omega)\big). \tag{3.3.3}$$

(ii) *If $m > \frac{n-1}{2}$, then the resolvent power difference in (3.3.3) is in the trace class, and for all $\lambda\in\rho(A_{\rm N})\cap\rho(A_{\rm D})$*

$$\begin{aligned}&\operatorname{tr}\Big((A_{\rm N}-\lambda)^{-m}-(A_{\rm D}-\lambda)^{-m}\Big)\\ &\qquad\qquad = \frac{1}{(m-1)!}\operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(M(\lambda)^{-1}M'(\lambda)\Big)\right).\end{aligned} \tag{3.3.4}$$

Proof. (i) We prove this item by applying Lemma 2.4. Fix an arbitrary $\lambda_0\in\mathbb{C}\setminus\mathbb{R}$ and let γ and M be as in Proposition 3.2. By Theorem 3.3 (ii) the resolvent difference of $A_{\rm D}$ and $A_{\rm N}$ at the point λ_0 can be written in the form

$$(A_{\rm D}-\lambda_0)^{-1}-(A_{\rm N}-\lambda_0)^{-1} = -\gamma(\lambda_0)M(\lambda_0)^{-1}\gamma(\overline{\lambda}_0)^*.$$

Furthermore, by Proposition 3.2 (ii) the operator $M(\lambda_0)$ is bijective and closed as an operator from $L^2(\partial\Omega)$ onto $H^1(\partial\Omega)$. Hence, $\operatorname{dom}\big(M(\lambda_0)^{-1}\big) = H^1(\partial\Omega)$ and, since $M(\lambda_0)^{-1}$ is closed as an operator from $H^1(\partial\Omega)$ onto $L^2(\partial\Omega)$, we conclude that $M(\lambda_0)^{-1} \in \mathcal{B}\big(H^1(\partial\Omega), L^2(\partial\Omega)\big)$. Set

$$H := A_{\mathrm{D}}, \quad K := A_{\mathrm{N}}, \quad F_1 := -\gamma(\lambda_0), \quad F_2 := M(\lambda_0)^{-1}\gamma(\overline{\lambda}_0)^*.$$

Then Proposition 3.10 (b) and (c) imply that the assumptions in Lemma 2.4 are satisfied with

$$a = \frac{2}{n-1}, \quad b_1 = \frac{3/2}{n-1}, \quad b_2 = \frac{1/2}{n-1}, \quad r = +\infty.$$

Since $b = b_1 + b_2 - a = 0$, Lemma 2.4 implies that

$$(A_{\mathrm{D}} - \lambda)^{-m} - (A_{\mathrm{N}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}\big(L^2(\Omega)\big)$$

for all $\lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}})$ and all $m \in \mathbb{N}$.

(ii) The proof of this item is split into three steps.

Step 1. Let us introduce the operator-valued function

$$S(\lambda) := M(\lambda)^{-1}\gamma(\overline{\lambda})^*, \qquad \lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}}).$$

Note that the product is well defined since

$$\operatorname{ran}(\gamma(\overline{\lambda})^*) \subset H^1(\partial\Omega) = \operatorname{dom}(M(\lambda)^{-1}).$$

Since A_{D} is self-adjoint, it follows from Proposition 2.11 (iii) that $S(\lambda)$ is a bounded operator from $L^2(\Omega)$ to $L^2(\partial\Omega)$ for all $\lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}})$. We prove the following smoothing property for the derivatives of S:

$$\text{(3.3.5)} \quad u \in H^s_{\partial\Omega}(\Omega) \quad \Rightarrow \quad S^{(k)}(\lambda)u \in H^{s+2k+1/2}(\partial\Omega), \qquad s \geq 0,\ k \in \mathbb{N}_0,$$

by induction. Since $\gamma(\overline{\lambda})^*$ maps $H^s_{\partial\Omega}(\Omega)$ into $H^{s+3/2}(\partial\Omega)$ for $s \geq 0$ by Lemma 3.9 (ii) and $M(\lambda)^{-1}$ maps $H^{s+3/2}(\partial\Omega)$ into $H^{s+1/2}(\partial\Omega)$ by Lemma 3.9 (iv), relation (3.3.5) is true for $k = 0$. Now let $l \in \mathbb{N}_0$ and assume that (3.3.5) is true for every $k = 0, 1, \dots, l$. By (2.2.6), (2.2.8) and Lemma 2.12 (i), (iii) we have

$$\begin{aligned}
S'(\lambda)u &= \frac{d}{d\lambda}\big(M(\lambda)^{-1}\big)\gamma(\overline{\lambda})^*u + M(\lambda)^{-1}\frac{d}{d\lambda}\gamma(\overline{\lambda})^*u \\
&= -M(\lambda)^{-1}M'(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*u + M(\lambda)^{-1}\gamma(\overline{\lambda})^*(A_{\mathrm{N}} - \lambda)^{-1}u \\
&= -M(\lambda)^{-1}\gamma(\overline{\lambda})^*\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*u + S(\lambda)(A_{\mathrm{N}} - \lambda)^{-1}u \\
&= S(\lambda)(A_{\mathrm{N}} - \lambda)^{-1}u - S(\lambda)\gamma(\lambda)S(\lambda)u
\end{aligned}$$

for all $u \in L^2(\Omega)$. Hence, with the help of (2.2.6), (2.2.7) and Lemma 2.12 (ii), we obtain

$$
\begin{aligned}
S^{(l+1)}(\lambda) =& \frac{d^l}{d\lambda^l}\Big(S(\lambda)(A_{\mathrm{N}}-\lambda)^{-1} - S(\lambda)\gamma(\lambda)S(\lambda)\Big) \\
=& \sum_{\substack{p+q=l \\ p,q\geq 0}} \binom{l}{p} S^{(p)}(\lambda)\frac{d^q}{d\lambda^q}(A_{\mathrm{N}}-\lambda)^{-1} \\
& - \sum_{\substack{p+q+r=l \\ p,q,r\geq 0}} \frac{l!}{p!\,q!\,r!} S^{(p)}(\lambda)\gamma^{(q)}(\lambda)S^{(r)}(\lambda) \\
=& \sum_{\substack{p+q=l \\ p,q\geq 0}} \frac{l!}{p!} S^{(p)}(\lambda)(A_{\mathrm{N}}-\lambda)^{-(q+1)} \\
& - \sum_{\substack{p+q+r=l \\ p,q,r\geq 0}} \frac{l!}{p!\,r!} S^{(p)}(\lambda)(A_{\mathrm{N}}-\lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda).
\end{aligned} \tag{3.3.6}
$$

By the induction hypothesis, smoothing property (3.3.1) and Lemma 3.9 (i), we have, for $s \geq 0$ and $p, q \geq 0$, $p+q=l$,

$$
\begin{aligned}
& u \in H^s_{\partial\Omega}(\Omega) \\
\Longrightarrow \quad & (A_{\mathrm{N}}-\lambda)^{-(q+1)}u \in H^{s+2q+2}_{\partial\Omega}(\Omega) \\
\Longrightarrow \quad & S^{(p)}(\lambda)(A_{\mathrm{N}}-\lambda)^{-(q+1)}u \in H^{s+2q+2+2p+1/2}(\partial\Omega) = H^{s+2(l+1)+1/2}(\partial\Omega)
\end{aligned}
$$

and for $s \geq 0$ and $p, q, r \geq 0$, $p+q+r=l$,

$$
\begin{aligned}
& u \in H^s_{\partial\Omega}(\Omega) \\
\Longrightarrow \quad & S^{(r)}(\lambda)u \in H^{s+2r+1/2}(\partial\Omega) \\
\Longrightarrow \quad & \gamma(\lambda)S^{(r)}(\lambda)u \in H^{s+2r+1/2+3/2}_{\partial\Omega}(\Omega) \\
\Longrightarrow \quad & (A_{\mathrm{N}}-\lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda)u \in H^{s+2r+2+2q}_{\partial\Omega}(\Omega) \\
\Longrightarrow \quad & S^{(p)}(\lambda)(A_{\mathrm{N}}-\lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda)u \in H^{s+2r+2+2q+2p+1/2}(\partial\Omega) \\
& \qquad = H^{s+2(l+1)+1/2}(\partial\Omega),
\end{aligned}
$$

which, together with (3.3.6), shows (3.3.5) for $k = l+1$ and hence, by induction, for all $k \in \mathbb{N}_0$. Therefore, an application of Lemma 2.22 yields that

$$S^{(k)}(\lambda) \in \mathfrak{S}_{\frac{n-1}{2k+1/2},\infty}\big(L^2(\Omega), L^2(\partial\Omega)\big), \qquad k \in \mathbb{N}_0,\ \lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}}). \tag{3.3.7}$$

Step 2. Using Krein's formula from Theorem 3.3 (ii) and (2.2.6) we can write, for $m \in \mathbb{N}$ and $\lambda \in \rho(A_{\mathrm{N}}) \cap \rho(A_{\mathrm{D}})$,

$$\begin{aligned}
(A_{\mathrm{N}} - \lambda)^{-m} - (A_{\mathrm{D}} - \lambda)^{-m} &= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} \Big((A_{\mathrm{N}} - \lambda)^{-1} - (A_{\mathrm{D}} - \lambda)^{-1} \Big) \\
&= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} \big(\gamma(\lambda) S(\lambda) \big) \\
&= \frac{1}{(m-1)!} \sum_{\substack{p+q=m-1 \\ p,q \geq 0}} \binom{m-1}{p} \gamma^{(p)}(\lambda) S^{(q)}(\lambda). \qquad (3.3.8)
\end{aligned}$$

By Proposition 3.11 (i), (3.3.7) and Lemma 2.3 (i)

$$\gamma^{(p)}(\lambda) S^{(q)}(\lambda) \in \mathfrak{S}_{\frac{n-1}{2p+3/2},\infty} \cdot \mathfrak{S}_{\frac{n-1}{2q+1/2},\infty} = \mathfrak{S}_{\frac{n-1}{2(p+q)+2},\infty} = \mathfrak{S}_{\frac{n-1}{2m},\infty} \tag{3.3.9}$$

for p, q with $p + q = m - 1$.

Step 3. If $m > \frac{n-1}{2}$, then $\frac{n-1}{2m} < 1$ and, by Lemma 2.3 (iii) and (3.3.9), each term in the sum in (3.3.8) is a trace class operator and, by a similar argument, also $S^{(q)}(\lambda)\gamma^{(p)}(\lambda)$. Hence the resolvent power difference in (3.3.3) is a trace class operator, and we can apply the trace to (3.3.8) and use (2.1.10), (2.1.11) and Lemma 2.12 (iii) to obtain

$$
\begin{aligned}
&(m-1)!\,\mathrm{tr}\Big((A_{\mathrm{N}}-\lambda)^{-m}-(A_{\mathrm{D}}-\lambda)^{-m}\Big)\\
&= \mathrm{tr}\Bigg(\sum_{\substack{p+q=m-1\\ p,q\geq 0}}\binom{m-1}{p}\gamma^{(p)}(\lambda)S^{(q)}(\lambda)\Bigg)\\
&= \sum_{\substack{p+q=m-1\\ p,q\geq 0}}\binom{m-1}{p}\,\mathrm{tr}\Big(\gamma^{(p)}(\lambda)S^{(q)}(\lambda)\Big)\\
&= \sum_{\substack{p+q=m-1\\ p,q\geq 0}}\binom{m-1}{p}\,\mathrm{tr}\Big(S^{(q)}(\lambda)\gamma^{(p)}(\lambda)\Big)\\
&= \mathrm{tr}\Bigg(\sum_{\substack{p+q=m-1\\ p,q\geq 0}}\binom{m-1}{p}S^{(q)}(\lambda)\gamma^{(p)}(\lambda)\Bigg) = \mathrm{tr}\bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(S(\lambda)\gamma(\lambda)\Big)\bigg)\\
&= \mathrm{tr}\bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(M(\lambda)^{-1}\gamma(\overline{\lambda})^*\gamma(\lambda)\Big)\bigg) = \mathrm{tr}\bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(M(\lambda)^{-1}M'(\lambda)\Big)\bigg),
\end{aligned}
$$

which finishes the proof.

□

Remark 3.13. As the reader might note the proof of item (ii) in Theorem 3.12 includes also an alternative of item (i), which is slightly more complicated in the author's opinion.

The previous theorem has a direct application in the mathematical scattering theory. We consider the pair $\{A_{\mathrm{D}}, A_{\mathrm{N}}\}$ of self-adjoint operators as a scattering system. The next corollary shows that the wave operators for the scattering system $\{A_{\mathrm{D}}, A_{\mathrm{N}}\}$ exist in any space dimension. The trace formula is also provided.

Corollary 3.14. *Let A_{D} and A_{N} be the self-adjoint operators defined in* (3.1.6)*. The wave operators $W_{\pm}(A_{\mathrm{D}}, A_{\mathrm{N}})$ for the scattering pair $\{A_{\mathrm{D}}, A_{\mathrm{N}}\}$ exist and are complete, and hence the absolutely continuous parts of A_{D} and A_{N} are untarily equivalent.*

Proof. By Theorem 3.12 for integer $m > \frac{n-1}{2}$ the m-th powers difference of the resolvents of A_{D} and A_{N} is in the trace class and the claim follows from Theorem 2.27. □

Further we provide $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power difference of $A_{[B]}$ and A_{N}. In this case we observe faster convergence of singular values than in Theorem 3.12. Note that $A_{[B]}$ can also be the usual Robin Laplacian with a real-valued bounded coefficient in the boundary condition.

Theorem 3.15. *Let A_{N} be the self-adjoint operator as in (3.1.6). Let B be a bounded self-adjoint operator in $L^2(\partial\Omega)$ and let $A_{[B]}$ be the self-adjoint operator corresponding to B via (3.2.4). Then the following statements hold.*

(i) *For all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{N}})$ and all $m \in \mathbb{N}$*

$$(A_{[B]} - \lambda)^{-m} - (A_{\mathrm{N}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1},\infty}\big(L^2(\Omega)\big). \tag{3.3.10}$$

(ii) *If $m > \frac{n}{2} - 1$, then the resolvent power difference in (3.3.10) is in the trace class and, for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{N}})$*

$$\begin{aligned}
&\operatorname{tr}\Big((A_{[B]} - \lambda)^{-m} - (A_{\mathrm{N}} - \lambda)^{-m}\Big) \\
&\qquad = \frac{1}{(m-1)!}\operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(\big(I - BM(\lambda)\big)^{-1} BM'(\lambda)\Big)\right).
\end{aligned}$$

Proof. (i) We prove this item by applying Lemma 2.4. Fix an arbitrary $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and let γ, M be as in Proposition 3.2. By Theorem 3.5 the resolvent difference of $A_{[B]}$ and A_{N} can be written in the form

$$(A_{[B]} - \lambda_0)^{-1} - (A_{\mathrm{N}} - \lambda_0)^{-1} = \gamma(\lambda_0)\big(I - BM(\lambda_0)\big)^{-1} B\gamma(\overline{\lambda}_0)^*,$$

where $(I - BM(\lambda_0))^{-1}B \in \mathcal{B}\big(L^2(\partial\Omega)\big)$. By Proposition 3.10 (a) and (b) the assumptions in Lemma 2.4 are satisfied with

$$H = A_{[B]}, \quad K = A_{\mathrm{N}}, \quad F_1 = \gamma(\lambda_0), \quad F_2 = \big(I - BM(\lambda_0)\big)^{-1} B\gamma(\overline{\lambda}_0)^*,$$

and with

$$a = \frac{2}{n-1}, \quad b_1 = b_2 = \frac{3/2}{n-1}, \quad r = +\infty.$$

Since $b = b_1 + b_2 - a = \frac{1}{n-1}$, Lemma 2.1.14 implies the statement.

(ii) The formula in this item is proved in a more general form in Theorem 3.17 further, where one should set $B_2 = B$ and $B_1 = 0$. $\square$

Corollary 3.16. *Let A_{N} be the self-adjoint operator as in (3.1.6). Let B be a bounded self-adjoint operator in $L^2(\partial\Omega)$ and let $A_{[B]}$ be the self-adjoint operator corresponding to B via (3.2.4). Then the wave operators $W_\pm(A_{[B]}, A_{\mathrm{N}})$ for the scattering pair $\{A_{[B]}, A_{\mathrm{N}}\}$ exist and are complete, and hence the absolutely continuous parts of $A_{[B]}$ and A_{N} are unitarily equivalent.*

In the next theorem we prove $\mathfrak{S}_{p,\infty}$-properties of the resolvent power differences for the self-adjoint operators $A_{[B_1]}$ and $A_{[B_2]}$. It turns out that the singular values in this case also converge faster than in Theorem 3.12 and, under some conditions, faster than in Theorem 3.15. Furthermore, we provide the corresponding trace formulae, where the trace of the resolvent power difference of $A_{[B_1]}$ and $A_{[B_2]}$ is expressed in terms of the Weyl function, its derivative and the operators B_1 and B_2, cf. [BMN08, CGNZ12, GZ12] for one-dimensional Schrödinger operators and other finite-rank situations. We also mention that the special case of classical Robin boundary conditions, where B_1 and B_2 are multiplication operators with real-valued L^∞-functions, is contained in Theorem 3.17.

Theorem 3.17. *Let the self-adjoint operator A_{N} be as in (3.1.6). Let B_1 and B_2 be bounded self-adjoint operators in $L^2(\partial\Omega)$. Set*

$$t := \begin{cases} \frac{n-1}{q}, & \text{if} \quad B_1 - B_2 \in \mathfrak{S}_{q,\infty},\ q > 0, \\ 0, & \text{otherwise.} \end{cases}$$

Let $A_{[B_1]}$ and $A_{[B_2]}$ be the self-adjoint operators in $L^2(\Omega)$ corresponding via (3.2.4) to B_1 and B_2, respectively. Then the following statements hold.

(i) *For all $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]})$ and all $m \in \mathbb{N}$*

$$(A_{[B_2]} - \lambda)^{-m} - (A_{[B_1]} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+t+1},\infty}\big(L^2(\Omega)\big). \tag{3.3.11}$$

(ii) *If $m > \frac{n-t}{2} - 1$, then the resolvent power difference in (3.3.11) is a trace class operator and, for all $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \rho(A_{\mathrm{N}})$,*

$$\begin{aligned} &\mathrm{tr}\Big((A_{[B_2]} - \lambda)^{-m} - (A_{[B_1]} - \lambda)^{-m}\Big) \\ &\qquad = \frac{1}{(m-1)!}\,\mathrm{tr}\bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(U(\lambda)M'(\lambda)\Big)\bigg), \end{aligned} \tag{3.3.12}$$

where $U(\lambda) := \big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1}$.

Proof. (i) Let us fix $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and let γ and M be as in Proposition 3.2. By Theorem 3.6 for all $\lambda \in \rho(A_{[B_2]}) \cap \rho(A_{[B_1]}) \cap \rho(A_{\mathrm{N}})$

$$\begin{aligned} &(A_{[B_2]} - \lambda_0)^{-1} - (A_{[B_1]} - \lambda_0)^{-1} \\ &\qquad = \gamma(\lambda_0)\big(I - B_2 M(\lambda_0)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda_0)B_1\big)^{-1}\gamma(\overline{\lambda}_0)^*, \end{aligned}$$

where the operators $(I - B_2 M(\lambda_0))^{-1}$ and $(I - M(\lambda_0)B_1)^{-1}$ are bounded and closed in $L^2(\partial\Omega)$. Now Proposition 3.10 (a), (b) and Theorem 3.15 imply that the assumptions in Lemma 2.6 are satisfied with

$$
\begin{aligned}
&H = A_{[B_2]}, \quad K = A_{[B_1]}, \quad L = A_{\mathrm{N}},\\
&F_1 = \gamma(\lambda_0)\big(I - B_2 M(\lambda_0)\big)^{-1}, \quad F_2 = (B_2 - B_1)\big(I - M(\lambda_0)B_1\big)^{-1}\gamma(\overline{\lambda}_0)^*,
\end{aligned}
$$

and with

$$
a = \frac{2}{n-1}, \quad b_1 = \frac{3/2}{n-1}, \quad b_2 = \frac{3/2 + t}{n-1}, \quad r = +\infty.
$$

Lemma 2.6 yields the statement for all $\lambda \in \rho(A_{[B_2]}) \cap \rho(A_{[B_1]}) \cap \rho(A_{\mathrm{N}})$ and the points in the discrete set $\rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \sigma(A_{\mathrm{N}})$ can be included via contour integrals.

(ii) In order to shorten notation and to avoid the distinction of several cases, we set

$$
\mathfrak{A}_r := \begin{cases} \mathfrak{S}_{\frac{n-1}{r},\infty}\big(L^2(\partial\Omega)\big) & \text{if } r > 0,\\ \mathcal{B}\big(L^2(\partial\Omega)\big) & \text{if } r = 0. \end{cases}
$$

It follows from Lemma 2.3 (i) and the fact that $\mathfrak{S}_{p,\infty}(L^2(\partial\Omega))$, $p > 0$ is an ideal in $\mathcal{B}(L^2(\partial\Omega))$ that

$$
\mathfrak{A}_{r_1} \cdot \mathfrak{A}_{r_2} = \mathfrak{A}_{r_1 + r_2}, \qquad r_1, r_2 \geq 0. \tag{3.3.13}
$$

The assumption on the difference of B_1 and B_2 yields

$$
B_2 - B_1 \in \mathfrak{A}_t. \tag{3.3.14}
$$

The proof of item (ii) is divided into four steps.
Step 1. Let B be a bounded self-adjoint operator in $L^2(\partial\Omega)$ and set

$$
T(\lambda) := \big(I - BM(\lambda)\big)^{-1}, \qquad \lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{N}}),
$$

where $T(\lambda) \in \mathcal{B}(L^2(\partial\Omega))$ by Lemma 2.19. We show that

$$
T^{(k)}(\lambda) \in \mathfrak{A}_{2k+1}, \qquad k \in \mathbb{N}, \tag{3.3.15}
$$

by induction. Relation (2.2.8) implies that

$$
T'(\lambda) = T(\lambda)BM'(\lambda)T(\lambda), \tag{3.3.16}
$$

which is in $\mathfrak{A}_3$ by Proposition 3.11 (ii). Let $l \in \mathbb{N}$ and assume that (3.3.15) is true for every $k = 1, \dots, l$, which implies in particular that

$$T^{(k)}(\lambda) \in \mathfrak{A}_{2k}, \qquad k = 0, \dots, l. \tag{3.3.17}$$

Then

$$\begin{aligned} T^{(l+1)}(\lambda) &= \frac{d^l}{d\lambda^l}\Big(T(\lambda)BM'(\lambda)T(\lambda)\Big) \\ &= \sum_{\substack{p+q+r=l \\ p,q,r\geq 0}} \frac{l!}{p!\,q!\,r!} T^{(p)}(\lambda)BM^{(q+1)}(\lambda)T^{(r)}(\lambda) \end{aligned}$$

by (3.3.16) and (2.2.7). Relation (3.3.17), the boundedness of B, Proposition 3.11 (ii) and (3.3.13) imply that

$$T^{(p)}(\lambda)BM^{(q+1)}(\lambda)T^{(r)}(\lambda) \in \mathfrak{A}_{2p} \cdot \mathfrak{A}_{2(q+1)+1} \cdot \mathfrak{A}_{2r} = \mathfrak{A}_{2(l+1)+1}$$

since $p+q+r = l$. This shows (3.3.15) for $k = l+1$ and hence, by induction, for all $k \in \mathbb{N}$. Since $T(\lambda) \in \mathcal{B}(L^2(\partial\Omega))$, we have

$$T^{(k)}(\lambda) \in \mathfrak{A}_{2k}, \qquad k \in \mathbb{N}_0,\ \lambda \in \rho(A_{\mathrm{N}}), \tag{3.3.18}$$

and by similar considerations also

$$\frac{d^k}{d\lambda^k}\big(I - M(\lambda)B\big)^{-1} \in \mathfrak{A}_{2k}, \qquad k \in \mathbb{N}_0,\ \lambda \in \rho(A_{\mathrm{N}}). \tag{3.3.19}$$

Step 2. With B_1, B_2 as in the statement of the theorem set

$$T_1(\lambda) := \big(I - M(\lambda)B_1\big)^{-1} \quad \text{and} \quad T_2(\lambda) := \big(I - B_2M(\lambda)\big)^{-1}$$

for $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \rho(A_{\mathrm{N}})$. We can write $U(\lambda) = T_2(\lambda)(B_2 - B_1)T_1(\lambda)$ and hence

$$U^{(k)}(\lambda) = \frac{d^k}{d\lambda^k}\Big(T_2(\lambda)(B_2 - B_1)T_1(\lambda)\Big) = \sum_{\substack{p+q=k \\ p,q\geq 0}} \binom{k}{p} T_2^{(p)}(\lambda)(B_2 - B_1)T_1^{(q)}(\lambda).$$

By (3.3.18), (3.3.19) and (3.3.14), each term in the sum satisfies

$$T_2^{(p)}(\lambda)(B_2 - B_1)T_1^{(q)}(\lambda) \in \mathfrak{A}_{2p} \cdot \mathfrak{A}_t \cdot \mathfrak{A}_{2q} = \mathfrak{A}_{2k+t},$$

and hence

$$U^{(k)}(\lambda) \in \mathfrak{A}_{2k+t}, \qquad k \in \mathbb{N}_0,\ \lambda \in \rho(A_{\mathrm{N}}). \tag{3.3.20}$$

Step 3. By applying Theorem 3.6 to $A_{[B_1]}$ and $A_{[B_2]}$ we obtain that, for $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \rho(A_{\mathrm{N}})$,

$$\begin{aligned}&(A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1}\\&= \gamma(\lambda)\Big[\big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1}\Big]\gamma(\overline{\lambda})^* = \gamma(\lambda)U(\lambda)\gamma(\overline{\lambda})^*.\end{aligned}$$

Taking derivatives we get, for $m \in \mathbb{N}$,

$$\begin{aligned}&(A_{[B_2]} - \lambda)^{-m} - (A_{[B_1]} - \lambda)^{-m}\\&= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}}\Big((A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1}\Big)\\&= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}}\Big(\gamma(\lambda)U(\lambda)\gamma(\overline{\lambda})^*\Big)\\&= \frac{1}{(m-1)!} \sum_{\substack{p+q+r=m-1\\p,q,r\geq 0}} \frac{(m-1)!}{p!\,q!\,r!}\gamma^{(p)}(\lambda)U^{(q)}(\lambda)\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^*. \qquad (3.3.21)\end{aligned}$$

By Proposition 3.11 (i) and (3.3.20), each term in the sum satisfies

$$\gamma^{(p)}(\lambda)U^{(q)}(\lambda)\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^* \in \mathfrak{S}_{\frac{n-1}{2p+3/2},\infty} \cdot \mathfrak{S}_{\frac{n-1}{2q+t},\infty} \cdot \mathfrak{S}_{\frac{n-1}{2r+3/2},\infty} = \mathfrak{S}_{\frac{n-1}{2m+t+1},\infty}. \qquad (3.3.22)$$

Step 4. If $m > \frac{n-t}{2} - 1$, then $\frac{n-1}{2m+t+1} < 1$ and, by Lemma 2.3 (iii) and (3.3.22), all the terms in the sum in (3.3.21) are trace class operators, and the same is true if we change the order in the product in (3.3.22). Hence we can apply the trace to the expression in (3.3.21) and use (2.1.10), (2.1.11) and Lemma 2.12 (iii) to obtain

$$\begin{aligned}&(m-1)!\,\mathrm{tr}\Big((A_{[B_2]} - \lambda)^{-m} - (A_{[B_1]} - \lambda)^{-m}\Big)\\&= \mathrm{tr}\left(\sum_{\substack{p+q+r=m-1\\p,q,r\geq 0}} \frac{(m-1)!}{p!\,q!\,r!}\gamma^{(p)}(\lambda)U^{(q)}(\lambda)\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^*\right)\\&= \sum_{\substack{p+q+r=m-1\\p,q,r\geq 0}} \frac{(m-1)!}{p!\,q!\,r!}\,\mathrm{tr}\Big(\gamma^{(p)}(\lambda)U^{(q)}(\lambda)\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^*\Big)\\&= \sum_{\substack{p+q+r=m-1\\p,q,r\geq 0}} \frac{(m-1)!}{p!\,q!\,r!}\,\mathrm{tr}\Big(U^{(q)}(\lambda)\Big(\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^*\Big)\gamma^{(p)}(\lambda)\Big)\end{aligned}$$

$$= \operatorname{tr}\Bigg(\sum_{\substack{p+q+r=m-1\\ p,q,r\geq 0}} \frac{(m-1)!}{p!\,q!\,r!} U^{(q)}(\lambda)\Big(\frac{d^r}{d\lambda^r}\gamma(\overline{\lambda})^*\Big)\gamma^{(p)}(\lambda)\Bigg)$$
$$= \operatorname{tr}\Bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(U(\lambda)\gamma(\overline{\lambda})^*\gamma(\lambda)\Big)\Bigg) = \operatorname{tr}\Bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(U(\lambda)M'(\lambda)\Big)\Bigg),$$

which shows (3.3.12). □

Remark 3.18. As the reader might note the proof of item (ii) of Theorem 3.17 contains also an alternative proof of item (i) of the same theorem.

In the next corollary we provide results for the pair of $A_{[B]}$ and A_{D}.

Corollary 3.19. *Let the assumptions be as in Theorem 3.15 and let A_{D} be the self-adjoint operator as in (3.1.6). Then the following holds.*

(i) *For all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{D}})$ and all $m \in \mathbb{N}$.*

$$(A_{\mathrm{D}} - \lambda)^{-m} - (A_{[B]} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}\big(L^2(\Omega)\big). \tag{3.3.23}$$

(ii) *If $m > \frac{n-1}{2}$, then the resolvent power difference in (3.3.23) is a trace class operator, and, for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$,*

$$\operatorname{tr}\Big((A_{[B]}-\lambda)^{-m}-(A_{\mathrm{D}}-\lambda)^{-m}\Big) = \frac{1}{(m-1)!}\operatorname{tr}\Bigg(\frac{d^{m-1}}{d\lambda^{m-1}}\Big(V(\lambda)M'(\lambda)\Big)\Bigg) \tag{3.3.24}$$

where $V(\lambda) := \big(I - M(\lambda)B\big)^{-1}M(\lambda)^{-1}$.

Proof. (i) By Theorem 3.12 and Theorem 3.15

$$\begin{aligned} X_1(\lambda) &:= (A_{\mathrm{N}} - \lambda)^{-m} - (A_{\mathrm{D}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m},\infty}\big(L^2(\Omega)\big)\\ X_2(\lambda) &:= (A_{[B]} - \lambda)^{-m} - (A_{\mathrm{N}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1},\infty}\big(L^2(\Omega)\big). \end{aligned} \tag{3.3.25}$$

hold for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$. Note that $\mathfrak{S}_{\frac{n-1}{2m+1},\infty} \subset \mathfrak{S}_{\frac{n-1}{2m},\infty}$. Taking the difference we get the statement for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{D}}) \cap \rho(A_{\mathrm{N}})$ and the points in the discrete set $\rho(A_{[B]}) \cap \rho(A_{\mathrm{D}}) \cap \sigma(A_{\mathrm{N}})$ can be included via contour integrals.

(ii) If $m > \frac{n-1}{2}$, then $\frac{n-1}{2m} < 1$ and hence, by item (i) and Lemma 2.3 (iii), the operator in (3.3.23) is a trace class operator. Using Theorem 3.12 (ii) and Theorem 3.15 (ii) we obtain

$$\operatorname{tr}\Big((A_{[B]}-\lambda)^{-m}-(A_{\mathrm{D}}-\lambda)^{-m}\Big)=\operatorname{tr}\big(X_1(\lambda)+X_2(\lambda)\big)$$
$$=\frac{1}{(m-1)!}\operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\left[\Big(M(\lambda)^{-1}+\big(I-BM(\lambda)\big)^{-1}B\Big)M'(\lambda)\right]\right).$$

Since

$$M(\lambda)^{-1}+\big(I-BM(\lambda)\big)^{-1}B$$
$$=\big(I-BM(\lambda)\big)^{-1}\Big[\big(I-BM(\lambda)\big)+BM(\lambda)\Big]M(\lambda)^{-1}=V(\lambda),$$

this implies (3.3.24). □

3.4 Comments

The realizations of elliptic differential expressions with differential operators of appropriate orders in the boundary conditions have already been studied up to the end of 50s, see, e.g., Agmon, Douglis and Nirenberg [ADN59] and as well as the comments in [LM68, Section 2.10]. These boundary conditions are called *local*, because it is possible to define their meaning in a neighborhood of a point. Results on elliptic differential operators and solvability of elliptic boundary value problems with more general *non-local* boundary conditions go back to the seminal paper by Vishik [V52] and then were followed by the works of Bade and Freeman [BF62], Freeman [F62] and Beals [Be65]. In particular, in [BF62, F62, Be65] certain subfamilies of closed realizations were parametrized. This progress was accompanied by the development of the abstract extension theory due to Calkin [C39], Krein [K47], Vishik [V52] and Birman [B56] and by the results in the theory of elliptic boundary value problems published by Lions and Magenes in the works from 1960 to 1963 and collected in [LM68]. Using these two theories Grubb [G68] parameterized all closed realizations of a given elliptic differential expression via operators acting on the boundary and solved the converse problem of finding the boundary operator for a given closed realization.

In the recent past the Weyl function for elliptic differential operators was introduced, which is a generalization of the Titchmarsh-Weyl coefficient well-known in Sturm-Liouville theory. This notion and the corresponding new operator-theoretical methods gave a new impulse for the investigation of elliptic differential operators with general boundary conditions. Amrein and

Pearson [AP04] introduced an analogue of the Titchmarsh-Weyl function for Schrödinger operators on three-dimensional exterior domains. Soon after that there appeared the works on symmetric elliptic differential expressions on general smooth domains by Behrndt and Langer [BL07], Post [Po07], Ryzhov [R07] and Alpay and Behrndt [AB09], where the Weyl function was defined as the well-known Neumann-to-Dirichlet or Dirichlet-to-Neumann maps and used together with Krein's formula for spectral analysis. Using the approach of [BL07], Behrndt and Rohleder extended in [BR12] some results of the classical Titchmarsh-Weyl theory to the case of Schrödinger operators on exterior domains.

Recently also an analogue of the Weyl function was introduced for non-symmetric differential expressions and a corresponding Krein-type formula was provided, see Brown, Marletta, Naboko, and Wood [BMNW08], Brown, Grubb and Wood [BGW09] and Malamud [M10]. Note that Weyl functions in the non-symmetric case were introduced earlier in the abstract setting by Malamud and Mogilevskii in [MM02]. Weyl functions and Krein's formulae in the case of non-smooth domains were given by Gesztesy and Mitrea [GM08, GM08a, GM11], Grubb [G08], Posilicano and Raimondi [PR09], and Abels, Grubb, and Wood [AGW10].

Schatten-von Neumann estimates for resolvent power differences of elliptic differential operators have a long history in spectral theory. The estimates in Theorem 3.12 (i) and Corollary 3.19 (i) in the case that $\mathcal{L}$ is a Schrödinger differential expression $-\Delta + q$ with a real-valued, possibly unbounded potential q on an exterior domain $\Omega \subset \mathbb{R}^3$ go back to the pioneering paper by Povzner [P53]. In that paper the operator in the boundary condition was a multiplication operator with a real-valued bounded function β. Povzner proved in [P53, Theorem 1.4] that

$$(A_{[\beta]} - \lambda)^{-1} - (A_{\mathrm{D}} - \lambda)^{-1} \in \mathfrak{S}_2(L^2(\Omega)).$$

His proof heavily depends on the space dimension and on the special form of the differential expression.

Using variational methods, Birman [B62] improved and extended the result of Povzner to arbitrary space dimensions, general elliptic differential expressions and also to mixed Robin-Dirichlet boundary conditions. The estimates in Theorem 3.12 (i) and Corollary 3.19 are encompassed by [B62, Theorem 2.3] in the case of $m = 1$. It was shown by Birman and Solomyak in [BS80, Theorem 3], see also [BS79], that the singular values for the resolvent difference ($m = 1$) in Theorem 3.12 (i) have an asymptotic behavior such that this resolvent difference can not belong to a better class in the scale of weak Schatten-von Neumann classes.

In the case that B_1 and B_2 are multiplication operators or more general pseudo-differential operators of certain orders the estimate in Theorem 3.17 (i) follows from the spectral theory of singular Green operators developed by Grubb in [G84, G12]. Using this theory she obtained in [G84, Theorem 5.1], see also [G74, G84a], the asymptotic behavior of singular values for the resolvent power difference in Theorem 3.12 (i). Later in [G11a, Theorem 3.5] and [G12a] the asymptotic behavior of singular values for the resolvent power difference in Theorem 3.17 (i) was provided in the case of multiplication operators B_1 and B_2 with additional smoothness of the coefficients. Schatten-von Neumann estimates in the case of non-local boundary conditions are also contained in [M10] by Malamud. In particular, the estimate in Corollary 3.19 (ii) is partially covered by [M10, Proposition 4.9].

Already sixty years ago a reduction formula of the type given in Subsection 3.3.2 appeared in the paper [JP51] by Jost and Pais, where the perturbation determinant for a Schrödinger operator on an interval was reduced to the boundary. A multi-dimensional Jost-Pais formula was proved recently by Gesztesy, Mitrea and Zinchenko in [GMZ07]. The trace formula in Theorem 3.12 (ii) is contained in the paper [Ca02, Théorème 2.2] by Carron in a slightly different context. The trace formulae in Theorems 3.15, 3.17 and Corollary 3.19 are new to the best of the author's knowledge. Their analogues for one-dimensional operators were shown recently, see [CGNZ12, GZ12].

The results on $\mathfrak{S}_p$-estimates of resolvent differences contained in the works of the author [BLL$^+$10, BLL12] were applied by Mugnolo and Nittka in [MN12, Theorem 4.3] to convergence of semigroups in $\mathfrak{S}_p$-norms.

Chapter 4

Schrödinger operators with δ and δ'-potentials supported on hypersurfaces

In this chapter self-adjoint Schrödinger operators with δ and δ'-interactions supported on compact smooth hypersurfaces are defined explicitly via their action and domain and also implicitly via sesquilinear forms. We show that both ways of definition lead to the same self-adjoint operators. It is worth mentioning that our definitions of surface δ and δ'-interactions are also compatible with the definitions of point δ and δ'-interactions in the one-dimensional case [AGHH05, AK00].

In the case of δ-interactions the sesquilinear form approach was already known [BEKS94] and has been used in many papers, e.g., [EK03, EY02, EY04, KV07], while the explicit way of definition is new. In the case of δ'-interactions for general hypersurfaces no rigorous approach has been developed until now, see [E08, Open Problem 7.2].

The main advantage of the definition via action and domain is that the regularity of the functions in the operator domain is given explicitly, which is important in many applications. Whereas in the definition via sesquilinear forms this regularity is hidden in the form. In particular, we provide a sufficient condition for H^2-regularity of the operator domains.

As the main problem of this chapter we study Schatten-von Neumann properties of the resolvent power differences of the free Schrödinger operator and Schrödinger operators with surface interactions. We prove better convergence of the singular values in some cases. As a direct consequence of Schatten-von Neumann estimates for resolvent power differences we get the existence and completeness of the wave operators for the corresponding scattering pairs. At the end of this chapter we also prove finiteness of the negative spectra for the Schrödinger operators with surface δ and δ'-interactions. Most of the results of this chapter are contained in the work of the author [BLL12a].

4.1 Preliminaries

Let $\Sigma \subset \mathbb{R}^n$, $n \geq 2$, be a compact connected C^∞-smooth hypersurface, which separates the Euclidean space $\mathbb{R}^n$ into a bounded interior domain $\Omega_{\rm i}$ and an unbounded exterior domain $\Omega_{\rm e}$. In particular, the hypersurface Σ coincides with the boundaries $\partial\Omega_{\rm i}$ and $\partial\Omega_{\rm e}$ of the interior and exterior domains. We often decompose a function $f \in L^2(\mathbb{R}^n) = L^2(\Omega_{\rm i}) \oplus L^2(\Omega_{\rm e})$ in the form $f = f_{\rm i} \oplus f_{\rm e}$, where $f_{\rm i} = f \upharpoonright \Omega_{\rm i}$ and $f_{\rm e} = f \upharpoonright \Omega_{\rm e}$. We agree to denote by $(\cdot,\cdot)$, $(\cdot,\cdot)_{\rm i}$, $(\cdot,\cdot)_{\rm e}$ and $(\cdot,\cdot)_\Sigma$ the inner products in the Hilbert spaces $L^2(\mathbb{R}^n)$, $L^2(\Omega_{\rm i})$, $L^2(\Omega_{\rm e})$ and $L^2(\Sigma)$, respectively. When it is clear from the context, we denote the inner products in the Hilbert spaces $L^2(\mathbb{R}^n;\mathbb{C}^n)$, $L^2(\Omega_{\rm i};\mathbb{C}^n)$, and $L^2(\Omega_{\rm e};\mathbb{C}^n)$ of vector-valued functions also by $(\cdot,\cdot)$, $(\cdot,\cdot)_{\rm i}$ and $(\cdot,\cdot)_{\rm e}$, respectively.

Throughout this chapter we deal with the Schrödinger differential expression

$$\mathcal{L} := -\Delta + V, \tag{4.1.1}$$

where $V\colon \mathbb{R}^n \to \mathbb{R}$ is a bounded potential. By $\mathcal{L}_{\rm i}$ and $\mathcal{L}_{\rm e}$ we denote the restrictions of the differential expression $\mathcal{L}$ onto $\Omega_{\rm i}$ and $\Omega_{\rm e}$, respectively. With the notation $V_{\rm i} := V \upharpoonright \Omega_{\rm i}$ and $V_{\rm e} :=\upharpoonright \Omega_{\rm e}$ we can clarify that $\mathcal{L}_{\rm i}$ acts on $\Omega_{\rm i}$ as $-\Delta + V_{\rm i}$ and that $\mathcal{L}_{\rm e}$ acts on $\Omega_{\rm e}$ as $-\Delta + V_{\rm e}$.

It is convenient to deal with the spaces

$$\begin{aligned} H^s_\Delta(\Omega_{\rm i}) &:= \big\{ f_{\rm i} \in H^s(\Omega_{\rm i})\colon \Delta f_{\rm i} \in L^2(\Omega_{\rm i}) \big\}, \quad s \geq 0, \\ H^s_\Delta(\Omega_{\rm e}) &:= \big\{ f_{\rm e} \in H^s(\Omega_{\rm e})\colon \Delta f_{\rm e} \in L^2(\Omega_{\rm e}) \big\}, \quad s \geq 0. \end{aligned}$$

For $s \geq 0$ we use short notations

$$H^s(\mathbb{R}^n\backslash\Sigma) := H^s(\Omega_{\rm i}) \oplus H^s(\Omega_{\rm e}), \quad H^s_\Delta(\mathbb{R}^n\backslash\Sigma) := H^s_\Delta(\Omega_{\rm i}) \oplus H^s_\Delta(\Omega_{\rm e}). \tag{4.1.2}$$

For a function $f \in H^s_\Delta(\mathbb{R}^n \setminus \Sigma)$ with $s \geq 0$ we denote by $f_{\rm i}|_\Sigma$ and $f_{\rm e}|_\Sigma$ its traces from both sides of Σ and we denote by $\partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma$ and $\partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma$ its traces of normal derivatives from both sides of Σ with normals pointing outwards Ω_{i} and Ω_{e}, respectively. For $s > 3/2$ the mapping

$$H^s(\mathbb{R}^n \setminus \Sigma) \ni f \mapsto \big\{ f_{\mathrm{i}}|_\Sigma, f_{\mathrm{e}}|_\Sigma, \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma, \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma \big\} \tag{4.1.3}$$

is well-defined and surjective onto $(H^{s-1/2}(\Sigma))^2 \times (H^{s-3/2}(\Sigma))^2$, and for $s \in [0,2)$ the mapping

$$H^s_\Delta(\mathbb{R}^n \setminus \Sigma) \ni f \mapsto \big\{ f_{\mathrm{i}}|_\Sigma, f_{\mathrm{e}}|_\Sigma, \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma, \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma \big\} \tag{4.1.4}$$

is also well-defined as the mapping into $(H^{s-1/2}(\Sigma))^2 \times (H^{s-3/2}(\Sigma)^2$. Separately, the mappings

$$\begin{aligned} &H^s_\Delta(\mathbb{R}^n \setminus \Sigma) \ni f \mapsto \{ f_{\mathrm{i}}|_\Sigma, f_{\mathrm{e}}|_\Sigma \}, \\ &H^s_\Delta(\mathbb{R}^n \setminus \Sigma) \ni f \mapsto \{ \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma, \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma \} \end{aligned}$$

are surjective onto $(H^{s-1/2}(\Sigma))^2$ and onto $(H^{s-3/2}(\Sigma))^2$, respectively.

We denote by $H^s_\Sigma(\Omega_{\mathrm{i}})$ and $H^s_\Sigma(\Omega_{\mathrm{e}})$ with $s \ge 0$ the subspaces of $L^2(\Omega_{\mathrm{i}})$ and $L^2(\Omega_{\mathrm{e}})$, respectively, defined as in (2.3.2) with $\partial\Omega = \Sigma$, and $\Omega = \Omega_{\mathrm{i}}$ or $\Omega = \Omega_{\mathrm{e}}$, respectively. Then we define certain mixed regularity spaces consisting of L^2-functions on $\mathbb{R}^n$, which belong to H^s in a neighborhood of Σ or both one-sided neighborhoods of Σ, respectively, i.e.,

$$\begin{aligned} H^s_\Sigma(\mathbb{R}^n) &:= \Big\{ f \in L^2(\mathbb{R}^n) \colon \exists \text{ domain } \Omega' \subset \mathbb{R}^n \text{ such that} \\ &\qquad\qquad \Omega' \supset \Sigma \text{ and } f \upharpoonright \Omega' \in H^s(\Omega') \Big\}, \\ H^s_\Sigma(\mathbb{R}^n \setminus \Sigma) &:= H^s_\Sigma(\Omega_{\mathrm{i}}) \oplus H^s_\Sigma(\Omega_{\mathrm{e}}). \end{aligned} \tag{4.1.5}$$

It is worth mentioning that $H^s_\Sigma(\mathbb{R}^n) \subsetneq H^s_\Sigma(\mathbb{R}^n \setminus \Sigma)$ for $s > 0$.

For $k \in \mathbb{N}_0$ we denote by $W^{k,\infty}_\Sigma(\Omega_{\mathrm{i}})$ and $W^{k,\infty}_\Sigma(\Omega_{\mathrm{e}})$, respectively, the subspaces of $L^\infty(\Omega_{\mathrm{i}})$ and $L^\infty(\Omega_{\mathrm{e}})$, defined as in (2.3.3) with $\partial\Omega = \Sigma$ and $\Omega = \Omega_{\mathrm{i}}$ or $\Omega = \Omega_{\mathrm{e}}$. We also make use of certain mixed regularity spaces consisting of L^∞-functions on $\mathbb{R}^n$ which belong to $W^{k,\infty}$ in a neighborhood of Σ or both one-sided neighborhoods of Σ. Namely,

$$\begin{aligned} W^{k,\infty}_\Sigma(\mathbb{R}^n) &:= \Big\{ f \in L^\infty(\mathbb{R}^n) \colon \exists \text{ domain } \Omega' \subset \mathbb{R}^n \text{ such that} \\ &\qquad\qquad \Omega' \supset \Sigma \text{ and } f \upharpoonright \Omega' \in W^{k,\infty}(\Omega') \Big\}, \\ W^{k,\infty}_\Sigma(\mathbb{R}^n \setminus \Sigma) &:= W^{k,\infty}_\Sigma(\Omega_{\mathrm{i}}) \times W^{k,\infty}_\Sigma(\Omega_{\mathrm{e}}). \end{aligned} \tag{4.1.6}$$

It is worth mentioning that $W^{k,\infty}_\Sigma(\mathbb{R}^n) \subsetneq W^{k,\infty}_\Sigma(\mathbb{R}^n \setminus \Sigma)$ for $k \in \mathbb{N}$.

For $f, g \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma)$ and $h \in H^1(\mathbb{R}^n \setminus \Sigma)$ the following first and second Green's identities hold:

$$(\mathcal{L}f, h) = \big(\nabla f, \nabla h\big) + \big(Vf, h\big) - \big(\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma, g_\mathrm{i}|_\Sigma\big)_\Sigma - \big(\partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma, g_\mathrm{e}|_\Sigma\big)_\Sigma \tag{4.1.7}$$

and

$$\begin{aligned}\big(\mathcal{L}f, g\big) - \big(f, \mathcal{L}g\big) = &\Big(\big(f_\mathrm{i}|_\Sigma, \partial_{\nu_\mathrm{i}} g_\mathrm{i}|_\Sigma\big)_\Sigma - \big(\partial_{\nu_\mathrm{i}} f|_\Sigma, g|_\Sigma\big)_\Sigma\Big) \\ &+ \Big(\big(f_\mathrm{e}|_\Sigma, \partial_{\nu_\mathrm{e}} g_\mathrm{e}|_\Sigma\big)_\Sigma - \big(\partial_{\nu_\mathrm{e}} f|_\Sigma, g_\mathrm{e}|_\Sigma\big)_\Sigma\Big).\end{aligned} \tag{4.1.8}$$

The minimal operators associated with the differential expressions $\mathcal{L}_\mathrm{i}$ and $\mathcal{L}_\mathrm{e}$ are defined by

$$\begin{aligned} A_\mathrm{i} f_\mathrm{i} &:= \mathcal{L}_\mathrm{i} f_\mathrm{i}, \qquad \operatorname{dom} A_\mathrm{i} := H^2_0(\Omega_\mathrm{i}), \\ A_\mathrm{e} f_\mathrm{e} &:= \mathcal{L}_\mathrm{e} f_\mathrm{e}, \qquad \operatorname{dom} A_\mathrm{e} := H^2_0(\Omega_\mathrm{e}). \end{aligned}$$

The operators A_i and A_e are densely defined, closed and symmetric with infinite deficiency indices, acting in the Hilbert spaces $L^2(\Omega_\mathrm{i})$ and $L^2(\Omega_\mathrm{e})$, respectively, with the adjoints of the form

$$\begin{aligned} A^*_\mathrm{i} f_\mathrm{i} &:= \mathcal{L}_\mathrm{i} f_\mathrm{i}, \qquad \operatorname{dom} A^*_\mathrm{i} := H^0_\Delta(\Omega_\mathrm{i}), \\ A^*_\mathrm{e} f_\mathrm{e} &:= \mathcal{L}_\mathrm{e} f_\mathrm{e}, \qquad \operatorname{dom} A^*_\mathrm{e} := H^0_\Delta(\Omega_\mathrm{e}). \end{aligned}$$

The direct sum of A_i and A_e

$$A_{\mathrm{i,e}} := A_\mathrm{i} \oplus A_\mathrm{e}, \qquad \operatorname{dom} A_{\mathrm{i,e}} := H^2_0(\Omega_\mathrm{i}) \oplus H^2_0(\Omega_\mathrm{e}), \tag{4.1.9}$$

is a densely defined, closed, symmetric operator with infinite deficiency indices in the Hilbert space $L^2(\mathbb{R}^n) = L^2(\Omega_\mathrm{i}) \oplus L^2(\Omega_\mathrm{e})$ and with the adjoint of the form

$$A^*_{\mathrm{i,e}} = \mathcal{L}f, \qquad \operatorname{dom} A^*_{\mathrm{i,e}} = H^0_\Delta(\mathbb{R}^n \setminus \Sigma).$$

Furthermore, we introduce the operators

$$\begin{aligned} T_\mathrm{i} f_\mathrm{i} &:= \mathcal{L}_\mathrm{i} f_\mathrm{i}, \qquad \operatorname{dom} T_\mathrm{i} := H^{3/2}_\Delta(\Omega_\mathrm{i}), \\ T_\mathrm{e} f_\mathrm{e} &:= \mathcal{L}_\mathrm{e} f_\mathrm{e}, \qquad \operatorname{dom} T_\mathrm{e} := H^{3/2}_\Delta(\Omega_\mathrm{e}), \end{aligned}$$

and their direct sum

$$T_{\mathrm{i,e}} := T_\mathrm{i} \oplus T_\mathrm{e}, \qquad \operatorname{dom} T_{\mathrm{i,e}} = H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma).$$

It can be shown that $A_{\rm i}^* = \overline{T}_{\rm i}$, $A_{\rm e}^* = \overline{T}_{\rm e}$, and hence $A_{\rm i,e}^* = \overline{T}_{\rm i,e}$.

Next we define usual self-adjoint Dirichlet and Neumann realizations of the differential expressions $\mathcal{L}_{\rm i}$ and $\mathcal{L}_{\rm e}$ in $L^2(\Omega_{\rm i})$ and $L^2(\Omega_{\rm e})$, respectively:

$$\begin{aligned}
A_{\rm D,i} f_{\rm i} &:= \mathcal{L}_{\rm i} f_{\rm i}, &\qquad \operatorname{dom} A_{\rm D,i} &:= \big\{ f_{\rm i} \in H^2(\Omega_{\rm i}) \colon f_{\rm i}|_\Sigma = 0 \big\},\\
A_{\rm D,e} f_{\rm e} &:= \mathcal{L}_{\rm e} f_{\rm e}, &\qquad \operatorname{dom} A_{\rm D,e} &:= \big\{ f_{\rm e} \in H^2(\Omega_{\rm e}) \colon f_{\rm e}|_\Sigma = 0 \big\},\\
A_{\rm N,i} f_{\rm i} &:= \mathcal{L}_{\rm i} f_{\rm i}, &\qquad \operatorname{dom} A_{\rm N,i} &:= \big\{ f_{\rm i} \in H^2(\Omega_{\rm i}) \colon \partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma = 0 \big\},\\
A_{\rm N,e} f_{\rm e} &:= \mathcal{L}_{\rm e} f_{\rm e}, &\qquad \operatorname{dom} A_{\rm N,e} &:= \big\{ f_{\rm e} \in H^2(\Omega_{\rm e}) \colon \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma = 0 \big\}.
\end{aligned}$$

Further, we define direct sums

$$\begin{aligned}
A_{\rm D,i,e} &:= A_{\rm D,i} \oplus A_{\rm D,e},\\
\operatorname{dom} A_{\rm D,i,e} &:= \big\{ f \in H^2(\mathbb{R}^n \setminus \Sigma) : f_{\rm i}|_\Sigma = f_{\rm e}|_\Sigma = 0 \big\},
\end{aligned} \tag{4.1.10}$$

and

$$\begin{aligned}
A_{\rm N,i,e} &:= A_{\rm N,i} \oplus A_{\rm N,e},\\
\operatorname{dom} A_{\rm N,i,e} &:= \big\{ f \in H^2(\mathbb{R}^n \setminus \Sigma) : \partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma = \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma = 0 \big\},
\end{aligned} \tag{4.1.11}$$

which are self-adjoint operators in $L^2(\mathbb{R}^n)$. Finally, we denote the usual self-adjoint (free) realization of $\mathcal{L}$ in $L^2(\mathbb{R}^n)$ by

$$A_{\rm free} f := \mathcal{L} f, \qquad \operatorname{dom} A_{\rm free} := H^2(\mathbb{R}^n). \tag{4.1.12}$$

One can associate quasi boundary triples $\Pi_{\rm i}$ and $\Pi_{\rm e}$ with the adjoints $A_{\rm i}^*$ and $A_{\rm e}^*$ as in Proposition 3.1. Denote the corresponding Weyl functions as in Proposition 3.2 by $M_{\rm i}$ and $M_{\rm e}$. These functions are well-defined on $\rho(A_{\rm N,i})$ and $\rho(A_{\rm N,e})$, respectively. For $\varphi \in L^2(\Sigma)$ and $\lambda \in \rho(A_{\rm N,j})$ with ${\rm j} = {\rm i}, {\rm e}$ the boundary value problem

$$\begin{aligned}
(\mathcal{L}_{\rm j} - \lambda) f_{\rm j} &= 0, \quad \text{in } \Omega_{\rm j},\\
\partial_{\nu_{\rm j}} f_{\rm j}|_\Sigma &= \varphi, \quad \text{on } \Sigma,
\end{aligned}$$

is uniquely solvable in $H^{3/2}_\Delta(\Omega_{\rm j})$. Denote its unique solution by $f_{\lambda,{\rm j}}$, then

$$M_{\rm j}(\lambda)\varphi = f_{\lambda,{\rm j}}|_\Sigma, \quad {\rm j} = {\rm i}, {\rm e}. \tag{4.1.13}$$

The operators $M_{\rm i}(\lambda)$ and $M_{\rm e}(\lambda)$ are, in fact, the Neumann-to-Dirichlet maps associated with the differential expressions $\mathcal{L}_{\rm i} - \lambda$ and $\mathcal{L}_{\rm e} - \lambda$, respectively.

4.2 Schrödinger operators with δ-potentials on hypersurfaces

In this section we use quasi boundary triples to define and study the Schrödinger operator $A_{\delta,\alpha}$ formally corresponding to the differential expression

$$\mathcal{L}_{\delta,\alpha} = -\Delta + V - \alpha \langle \delta_\Sigma, \cdot \rangle \, \delta_\Sigma,$$

where δ_Σ is the δ-distribution supported on Σ.

4.2.1 A quasi boundary triple and its Weyl function

It is convenient to define a quasi boundary triple not for $A_{\mathrm{i,e}}^*$ itself, but for the adjoint of a symmetric intermediate extension of $A_{\mathrm{i,e}}$. The method of intermediate extensions is inspired by the general considerations for ordinary boundary triples in [DHMS00, Section 4]. We define the extension

$$\widetilde{A} := A_{\mathrm{free}} \cap A_{\mathrm{D,i,e}} = \mathcal{L} \restriction \big\{ f \in H^2(\mathbb{R}^n)\colon f_{\mathrm{i}}|_\Sigma = f_{\mathrm{e}}|_\Sigma = 0 \big\} \tag{4.2.1}$$

of the orthogonal sum $A_{\mathrm{i,e}}$ in (4.1.9) as the underlying symmetric operator for the quasi boundary triple. Furthermore, we define the operator

$$\widetilde{T} := T_{\mathrm{i,e}} \restriction \big\{ f_{\mathrm{i}} \oplus f_{\mathrm{e}} \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma)\colon f_{\mathrm{i}}|_\Sigma = f_{\mathrm{e}}|_\Sigma \big\}, \tag{4.2.2}$$

and we specify the following two boundary mappings from $\operatorname{dom} \widetilde{T}$ into $L^2(\Sigma)$

$$\begin{aligned} &\widetilde{\Gamma}_0\colon \operatorname{dom} \widetilde{T} \to L^2(\Sigma), \quad \widetilde{\Gamma}_0 f := \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma + \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma, \\ &\widetilde{\Gamma}_1\colon \operatorname{dom} \widetilde{T} \to L^2(\Sigma), \quad \widetilde{\Gamma}_1 f := f_{\mathrm{i}}|_\Sigma = f_{\mathrm{e}}|_\Sigma. \end{aligned} \tag{4.2.3}$$

Note that the mappings $\widetilde{\Gamma}_0$, $\widetilde{\Gamma}_1$ are well defined because of the properties of the trace mappings (4.1.4).

In the first proposition of this section we prove that $\{L^2(\Sigma), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is a quasi boundary triple for $\widetilde{A}^*$ and we show basic properties of this triple.

Proposition 4.1. *Let the operators $A_{\mathrm{D,i,e}}$ and A_{free} be as in (4.1.10) and (4.1.12), respectively. Let the operators $\widetilde{A}$ and $\widetilde{T}$ and the mappings $\widetilde{\Gamma}_0$,$\widetilde{\Gamma}_1$ be, respectively, as in (4.2.1), (4.2.2) and (4.2.3). Then the triple $\widetilde{\Pi} = \{L^2(\Sigma), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is a quasi boundary triple for $\widetilde{A}^*$. The restrictions of $\widetilde{T}$ to the kernels of the boundary mappings are*

$$\widetilde{T} \restriction \ker \widetilde{\Gamma}_0 = A_{\mathrm{free}} \quad \textit{and} \quad \widetilde{T} \restriction \ker \widetilde{\Gamma}_1 = A_{\mathrm{D,i,e}};$$

and the ranges of these mappings are

$$\operatorname{ran}\widetilde{\Gamma}_0 = L^2(\Sigma) \quad \textit{and} \quad \operatorname{ran}\widetilde{\Gamma}_1 = H^1(\Sigma).$$

Proof. We show that the triple $\widetilde{\Pi}$ satisfies the conditions (a), (b) and (c) in Proposition 2.9. For the condition (a), let $\varphi \in H^{1/2}(\Sigma)$ and $\psi \in H^{3/2}(\Sigma)$ be arbitrary. By (3.1.2) there exist $f_\mathrm{i} \in H^2(\Omega_\mathrm{i})$ and $f_\mathrm{e} \in H^2(\Omega_\mathrm{e})$ such that

$$\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma = \varphi, \qquad f_\mathrm{i}|_\Sigma = \psi, \qquad \partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma = 0, \qquad f_\mathrm{e}|_\Sigma = \psi.$$

Since $H^2(\mathbb{R}^n\setminus\Sigma) \subset H^{3/2}_\Delta(\mathbb{R}^n\setminus\Sigma)$, we have $f := f_\mathrm{i}\oplus f_\mathrm{e} \in \operatorname{dom}\widetilde{T}$ and $\widetilde{\Gamma}_0 f = \varphi$, $\widetilde{\Gamma}_1 f = \psi$. Hence, we get

$$H^{1/2}(\Sigma) \times H^{3/2}(\Sigma) \subset \operatorname{ran}\begin{pmatrix}\widetilde{\Gamma}_0\\ \widetilde{\Gamma}_1\end{pmatrix}.$$

The set $H^{1/2}(\Sigma) \times H^{3/2}(\Sigma)$ is, clearly, dense in $L^2(\Sigma) \times L^2(\Sigma)$; note that also the set $\ker\widetilde{\Gamma}_0 \cap \ker\widetilde{\Gamma}_1$ is dense in $L^2(\mathbb{R}^n)$, which implies together that (a) of Proposition 2.9 is satisfied. Next let $f = f_\mathrm{i}\oplus f_\mathrm{e}$ and $g = g_\mathrm{i}\oplus g_\mathrm{e}$ be two arbitrary functions in $\operatorname{dom}\widetilde{T}$. Since the functions f and g in $\operatorname{dom}\widetilde{T}$ satisfy the boundary conditions $f_\mathrm{i}|_\Sigma = f_\mathrm{e}|_\Sigma = f|_\Sigma$ and $g_\mathrm{i}|_\Sigma = g_\mathrm{e}|_\Sigma = g|_\Sigma$, we have by Green's identity (4.1.8)

(4.2.4)
$$\big(\widetilde{T}f, g\big) - \big(f, \widetilde{T}g\big) = \big(f|_\Sigma, \partial_{\nu_\mathrm{i}} g_\mathrm{i}|_\Sigma + \partial_{\nu_\mathrm{e}} g_\mathrm{e}|_\Sigma\big)_\Sigma - \big(\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma + \partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma, g|_\Sigma\big)_\Sigma,$$

which shows that condition (b) of Proposition 2.9 is fulfilled. Since $\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_0$ contains the self-adjoint operator A_{free}, also the condition (c) is satisfied. Hence we can apply Proposition 2.9, which implies that $\widetilde{T} \upharpoonright (\ker\widetilde{\Gamma}_0 \cap \ker\widetilde{\Gamma}_1)$ is a densely defined closed symmetric operator and that the triple $\widetilde{\Pi} = \{L^2(\Sigma), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is a quasi boundary triple for its adjoint. Note that the operators and that $\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_0$ and $\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_1$ are symmetric by (4.2.4), and they contain self-adjoint operators A_{free} and $A_{\mathrm{D,i,e}}$, respectively. Therefore $\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_0 = A_{\mathrm{free}}$ and $\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_1 = A_{\mathrm{D,i,e}}$. Hence we get

$$\widetilde{T} \upharpoonright (\ker\widetilde{\Gamma}_0 \cap \ker\widetilde{\Gamma}_1) = \big(\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_0\big) \cap \big(\widetilde{T} \upharpoonright \ker\widetilde{\Gamma}_1\big) = A_{\mathrm{free}} \cap A_{\mathrm{D,i,e}} = \widetilde{A}.$$

Since, for $\mathrm{j} = \mathrm{i}$ and $\mathrm{j} = \mathrm{e}$, the mapping $f_\mathrm{j} \mapsto f_\mathrm{j}|_\Sigma$ is surjective from $H^{3/2}_\Delta(\Omega_j)$ onto $H^1(\Sigma)$ and the mapping $f_\mathrm{j} \mapsto \partial_{\nu_\mathrm{j}} f_\mathrm{j}|_\Sigma$ is surjective from $H^{3/2}_\Delta(\Omega_\mathrm{j})$ onto $L^2(\Sigma)$, it follows easily that $\operatorname{ran}\widetilde{\Gamma}_1 = H^1(\Sigma)$ and $\operatorname{ran}\widetilde{\Gamma}_0 \subset L^2(\Sigma)$. In order to see that $\widetilde{\Gamma}_0$ maps surjectively onto $L^2(\Sigma)$, let us fix an arbitrary $\chi \in C_0^\infty(\mathbb{R}^n)$ such that $\chi \equiv 1$ on an open neighbourhood of $\overline{\Omega_{\mathrm{i}}}$. Let SL be the single-layer potential associated with the hypersurface Σ and the differential expression $-\Delta+1$; see, e.g. [McL00, Chapter 6] for the definition and properties of single-layer potentials. By [McL00, Theorem 6.11, Theorem 6.12 (i)], for an arbitrary $\varphi \in L^2(\Sigma)$, the function $f := \chi\mathrm{SL}\varphi$ belongs to $\operatorname{dom}\widetilde{T}$ and satisfies the condition

$$\partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma + \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma = \varphi,$$

hence $\widetilde{\Gamma}_0 f = \varphi$, and thus $\operatorname{ran}\widetilde{\Gamma}_0 = L^2(\Sigma)$.

□

In the next proposition we clarify the basic properties of the γ-field and the Weyl function associated with the quasi boundary triple $\widetilde{\Pi}$ from Proposition 4.1. In the terminology of [McL00] the γ-field turns out to be the *single layer potential* associated with the hypersurface Σ and the differential expression $\mathcal{L} - \lambda$, see also Remark 4.3 after the proposition.

Proposition 4.2. *Let the self-adjoint operators $A_{\mathrm{D,i,e}}$ and A_{free} be as in (4.1.10) and (4.1.12), respectively. Let $\widetilde{\Pi}$ be the quasi boundary triple from Proposition 4.1. Let $\widetilde{\gamma}$ and $\widetilde{M}$ be the γ-field and the Weyl function associated with the quasi boundary triple $\widetilde{\Pi}$ as in Definition 2.10. Let M_{i} and M_{e} be the Weyl functions defined in (4.1.13). Then the following statements hold.*

(i) *The γ-field $\widetilde{\gamma}$ is defined for all $\lambda \in \rho(A_{\mathrm{free}})$ and*

$$\widetilde{\gamma}(\lambda)\colon L^2(\Sigma) \to L^2(\mathbb{R}^n), \qquad \widetilde{\gamma}(\lambda)\varphi = f_\lambda(\varphi),$$

where $f_\lambda(\varphi)$ is the unique solution in $H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma)$ of the problem

$$\begin{aligned} -\Delta f + Vf - \lambda f &= 0, \quad \text{in } \mathbb{R}^n \setminus \Sigma,\\ f_{\mathrm{i}}|_\Sigma = f_{\mathrm{e}}|_\Sigma &= 0, \quad \text{on } \Sigma,\\ \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma + \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma &= \varphi, \quad \text{on } \Sigma. \end{aligned}$$

(ii) *The Weyl function $\widetilde{M}$ is defined for all $\lambda \in \rho(A_{\mathrm{free}})$ and*

$$\widetilde{M}(\lambda)\colon L^2(\Sigma) \to L^2(\Sigma), \qquad \widetilde{M}(\lambda)\varphi = f_\lambda(\varphi)|_\Sigma,$$

where $f_\lambda(\varphi) = \widetilde{\gamma}(\lambda)\varphi$. For all $\lambda \in \rho(A_{\mathrm{free}})$ ($\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{D,i,e}})$) the operator $\widetilde{M}(\lambda)$ maps $L^2(\Sigma)$ into (onto) $H^1(\Sigma)$. The operator $\widetilde{M}(\lambda)$ is compact for all $\lambda \in \rho(A_{\mathrm{free}})$. Moreover, the identity

$$\widetilde{M}(\lambda) = \big(M_{\mathrm{i}}(\lambda)^{-1} + M_{\mathrm{e}}(\lambda)^{-1}\big)^{-1} \tag{4.2.5}$$

holds for all $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{D,i,e}}) \cap \rho(A_{\mathrm{N,i,e}})$.

Proof. (i) The mapping properties of the γ-field $\widetilde{\gamma}$ follow from (4.2.2), (4.2.3) and Definition 2.10.

(ii) The mapping properties of the Weyl function $\widetilde{M}$ follow from (4.2.3), Definition 2.10, Proposition 2.11 (iii) and Proposition 4.1. The compactness of the operator $\widetilde{M}(\lambda)$ follows from the compactness of the embedding of $H^1(\Sigma)$ into $L^2(\Sigma)$, cf. Lemma 2.22.

In order to prove the identity (4.2.5), let $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{D,i,e}}) \cap \rho(A_{\mathrm{N,i,e}})$. For such λ the operator $\widetilde{M}(\lambda)$ is invertible, and the same holds true for $M_{\mathrm{i}}(\lambda)$ and $M_{\mathrm{e}}(\lambda)$; cf. Proposition 3.2 and Theorem 2.13 (i). If $\widetilde{M}(\lambda)\varphi = \psi$ for some $\varphi \in L^2(\Sigma)$ and $\psi \in H^1(\Sigma)$, then there exists an $f = f_{\mathrm{i}} \oplus f_{\mathrm{e}} \in \ker(\widetilde{T} - \lambda)$ such that

$$\widetilde{\Gamma}_0 f = \varphi \qquad \text{and} \qquad \widetilde{\Gamma}_1 f = \psi.$$

As $f_{\mathrm{i}} \in \ker(T_{\mathrm{i}} - \lambda)$ and $f_{\mathrm{e}} \in \ker(T_{\mathrm{e}} - \lambda)$, we have

$$\begin{aligned} \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma &= M_{\mathrm{i}}(\lambda)^{-1}(f_{\mathrm{i}}|_\Sigma) = M_{\mathrm{i}}(\lambda)^{-1}\psi, \\ \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma &= M_{\mathrm{e}}(\lambda)^{-1}(f_{\mathrm{e}}|_\Sigma) = M_{\mathrm{e}}(\lambda)^{-1}\psi, \end{aligned}$$

and hence

$$\widetilde{M}(\lambda)^{-1}\psi = \varphi = \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma + \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma = M_{\mathrm{i}}(\lambda)^{-1}\psi + M_{\mathrm{e}}(\lambda)^{-1}\psi.$$

Since this is true for arbitrary $\psi \in H^1(\Sigma)$, relation (4.2.5) follows. □

We remark that the quasi boundary triple from Proposition 4.1 and the Weyl function above appear also implicitly in [AP04] and [R09, Section 4] in a different context.

Remark 4.3. Assume for simplicity that the potential V in the differential expression $\mathcal{L}$ in (4.1.1) is identically equal to zero. In this case the γ-field $\widetilde{\gamma}$ and the Weyl function $\widetilde{M}$ are, roughly speaking, extensions of the acoustic single-layer potential for the Helmholtz equation. In fact, if G_λ, $\lambda \in \mathbb{C} \setminus \mathbb{R}$, is the integral kernel of the resolvent of A_{free}, then for all $\varphi \in C^\infty(\Sigma)$ we have

$$\big(\widetilde{\gamma}(\lambda)\varphi\big)(x) = \int_\Sigma G_\lambda(x,y)\varphi(y)\,d\sigma_y, \quad x \in \mathbb{R}^n \setminus \Sigma,$$

and

$$\big(\widetilde{M}(\lambda)\varphi\big)(x) = \int_\Sigma G_\lambda(x,y)\varphi(y)\,d\sigma_y, \quad x \in \Sigma,$$

where σ_y is the natural Lebesgue measure on Σ. For more details we refer the reader to [McL00, Chapter 6]; see also [CK83, Co88].

4.2.2 Self-adjointness and Krein's formulae

In the first theorem of this subsection we establish a correspondence between the point spectra of the self-adjoint operator $A_{\mathrm{D,i,e}}$ and of the operator-valued function $\widetilde{M}(\cdot)$. Moreover, we provide a factorization (Krein's formula) for the resolvent difference of A_{free} and $A_{\mathrm{D,i,e}}$.

Theorem 4.4. *Let the self-adjoint operators $A_{\mathrm{D,i,e}}$ and A_{free} be as in (4.1.10) and (4.1.12). Let $\widetilde{\gamma}$ and $\widetilde{M}$ be the γ-field and the Weyl function from Proposition 4.2. Then the following statements hold.*

(i) *For all $\lambda \in \mathbb{R} \cap \rho(A_{\mathrm{free}})$*

$$\lambda \in \sigma_{\mathrm{p}}(A_{\mathrm{D,i,e}}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}(\widetilde{M}(\lambda))$$

and the multiplicities of these eigenvalues coincide.

(ii) *The formula*

$$(A_{\mathrm{free}} - \lambda)^{-1} - (A_{\mathrm{D,i,e}} - \lambda)^{-1} = \widetilde{\gamma}(\lambda)\widetilde{M}(\lambda)^{-1}\widetilde{\gamma}(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{\mathrm{D,i,e}}) \cap \rho(A_{\mathrm{free}})$.

Proof. The equivalence between the point spectra in item (i) and Krein's formula in item (ii) follow from the corresponding items of Theorem 2.13 with self-adjoint $A_0 = A_{\mathrm{free}}$ and $A_1 = A_{\mathrm{D,i,e}}$. □

We introduce a family of restrictions on the operator $\widetilde{T}$ parameterized by a bounded real-valued function on Σ.

Definition 4.5. For a real-valued function $\alpha \in L^\infty(\Sigma)$ the Schrödinger operator with δ-potential on the hypersurface Σ and strength α is defined as follows:

$$A_{\delta,\alpha} := \widetilde{T} \upharpoonright \ker(\alpha\widetilde{\Gamma}_1 - \widetilde{\Gamma}_0),$$

which is equivalent to

$$\begin{aligned} A_{\delta,\alpha} f &= -\Delta f + V f, \\ \operatorname{dom} A_{\delta,\alpha} &= \left\{ f \in H^{3/2}_{\Delta}(\mathbb{R}^n \setminus \Sigma) \colon \begin{array}{c} f_{\mathrm{i}}|_\Sigma = f_{\mathrm{e}}|_\Sigma = f|_\Sigma \\ \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma + \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma = \alpha f|_\Sigma \end{array} \right\}. \end{aligned} \tag{4.2.6}$$

The definition of $A_{\delta,\alpha}$ is compatible with the definition of a point δ-interaction in the one-dimensional case [AGHH05, Section I.3], [AK00] and the definitions of the operators with δ-potentials on hypersurfaces given in [AGS87, Sh88] and in [BEKS94]; see also Proposition 4.30. Note also that the domain of $A_{\delta,\alpha}$ is contained in $H^1(\mathbb{R}^n)$; cf. Proposition 4.30.

$$\overline{\overline{\widetilde{T}}} = \widetilde{A}^*$$

$$\overline{T}_{\mathrm{i,e}} = A_{\mathrm{i,e}}^*$$

$$\begin{tikzcd}
 & & A_{\mathrm{free}} \arrow[dr, hook] & & \\
A_{\mathrm{i,e}} \arrow[r, phantom, "\subset"] & \widetilde{A} \arrow[r, phantom, "\subset"] \arrow[ur, hook] \arrow[dr, hook] & A_{\delta,\alpha} \arrow[r, phantom, "\subset"] & \widetilde{T} \arrow[r, phantom, "\subset"] & T_{\mathrm{i,e}} \\
 & & A_{\mathrm{D,i,e}} \arrow[ur, hook] & &
\end{tikzcd}$$

Figure 4.1: This figure shows how the operator $A_{\delta,\alpha}$ is related to the other operators introduced in this section. The operators A_{free}, $A_{\delta,\alpha}$ and $A_{\mathrm{D,i,e}}$ are self-adjoint in $L^2(\mathbb{R}^n)$; cf. Theorem 4.6.

The next theorem contains the proof of self-adjointness of $A_{\delta,\alpha}$ and provides a factorization (Krein's formula) for the resolvent difference of $A_{\delta,\alpha}$ and A_{free}, cf. [BEKS94, Lemma 2.3 (iii)]. Item (ii) in Theorem 4.6 can be viewed as a variant of the Birman–Schwinger principle; it coincides with the one in [BEKS94].

Theorem 4.6. *Let $A_{\delta,\alpha}$ be as above and let A_{free} be the self-adjoint operator defined in (4.1.12). Let $\widetilde{\gamma}$ and $\widetilde{M}$ be the γ-field and the Weyl function from Proposition 4.2. Then the following statements hold.*

(i) *The operator $A_{\delta,\alpha}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R}^n)$.*

(ii) *For all $\lambda \in \mathbb{R} \cap \rho(A_{\mathrm{free}})$*

$$\lambda \in \sigma_{\mathrm{p}}(A_{\delta,\alpha}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}\big(I - \alpha \widetilde{M}(\lambda)\big)$$

and the multiplicities of these eigenvalues coincide.

(iii) *The formula*

$$(A_{\delta,\alpha} - \lambda)^{-1} - (A_{\mathrm{free}} - \lambda)^{-1} = \widetilde{\gamma}(\lambda) \left(I - \alpha \widetilde{M}(\lambda)\right)^{-1} \alpha \, \widetilde{\gamma}(\overline{\lambda})^*.$$

holds for all $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\rm free})$. In this formula the middle term on the right-hand side satisfies $(I - \alpha\widetilde{M}(\lambda))^{-1} \in \mathcal{B}(L^2(\Sigma))$.

Proof. (i) By Proposition 4.1 the range of the boundary mapping $\widetilde{\Gamma}_0$ coincides with $L^2(\Sigma)$. According to Proposition 4.2 the values of the Weyl function $\widetilde{M}$ are compact operators. By the assumptions on the function α the operator of multiplication with α is bounded and self-adjoint in $L^2(\Sigma)$ and the statement follows from Theorem 2.20.

(ii) The spectral equivalence follows from Proposition 2.14.

(iii) Krein's formula follows from self-adjointness of $A_{\delta,\alpha}$ and Corollary 2.16 with $A_0 = A_{\rm N}$ and $A_{[B]} = A_{\delta,\alpha}$. The property of the middle term follows from Lemma 2.19. □

Recall that the spaces $H^{3/2}_{\Delta}(\mathbb{R}^n \setminus \Sigma)$ and $H^2(\mathbb{R}^n \setminus \Sigma)$ are defined as in Section 4.1 and the space $W^{1,\infty}(\Sigma)$ is defined as in Section 2.3. It follows from Definition 4.5 that $\operatorname{dom} A_{\delta,\alpha} \subset H^{3/2}_{\Delta}(\mathbb{R}^n\setminus\Sigma)$. As in the previous chapter additional smoothness of the coefficient in the boundary condition leads to $\operatorname{dom} A_{\delta,\alpha} \subset H^2(\mathbb{R}^n \setminus \Sigma)$. In the next theorem we clarify this property.

Theorem 4.7. *Assume that a real-valued function α satisfies $\alpha \in W^{1,\infty}(\Sigma)$. Let the self-adjoint operator $A_{\delta,\alpha}$ be as in Definition 4.5. Then the inclusion* $\operatorname{dom} A_{\delta,\alpha} \subset H^2(\mathbb{R}^n \setminus \Sigma)$ *holds.*

Proof. For any function $f \in \operatorname{dom} A_{\delta,\alpha}$ we have $f \in \operatorname{dom} \widetilde{T} \subset H^{3/2}_{\Delta}(\mathbb{R}^n \setminus \Sigma)$. Then by Proposition 4.1 (i)

$$\widetilde{\Gamma}_1 f \in H^1(\Sigma).$$

The definition of the operator $A_{\delta,\alpha}$, the assumptions on the smoothness of α and the property (2.3.1) imply that

$$\widetilde{\Gamma}_0 f = \alpha\widetilde{\Gamma}_1 f \in H^1(\Sigma). \tag{4.2.7}$$

Let us fix $\lambda \in \mathbb{C} \setminus \mathbb{R}$. By the decomposition

$$\operatorname{dom} \widetilde{T} = \operatorname{dom} A_{\rm free} \dotplus \ker(\widetilde{T} - \lambda) \tag{4.2.8}$$

the function $f \in \operatorname{dom} A_{\delta,\alpha}$ can be represented as $f = f_{\rm free} + f_\lambda$ with $f_{\rm free} \in \operatorname{dom} A_{\rm free}$ and $f_\lambda \in \ker(\widetilde{T} - \lambda)$. It is clear that $f_{\rm free} \in H^2(\mathbb{R}^n) \subset H^2(\mathbb{R}^n \setminus \Sigma)$. The relation (4.2.7) and $A_{\rm free} = \widetilde{T} \upharpoonright \ker \widetilde{\Gamma}_0$ yield

$$\widetilde{\Gamma}_0 f_\lambda = \widetilde{\Gamma}_0 f \in H^1(\Sigma) \subset H^{1/2}(\Sigma). \tag{4.2.9}$$

The properties of the trace map in (4.1.3) show that $\widetilde{\Gamma}_0$ maps $\operatorname{dom}\widetilde{T} \cap H^2(\mathbb{R}^n \setminus \Sigma)$ onto $H^{1/2}(\Sigma)$, and hence (4.2.8) implies that $\widetilde{\Gamma}_0$ maps

$$\ker(\widetilde{T} - \lambda) \cap H^2(\mathbb{R}^n \setminus \Sigma)$$

bijectively onto $H^{1/2}(\Sigma)$. The last observation and (4.2.9) show that $f_\lambda \in H^2(\mathbb{R}^n \setminus \Sigma)$, and therefore $f = f_{\mathrm{free}} + f_\lambda \in H^2(\mathbb{R}^n \setminus \Sigma)$. $\square$

4.3 Schrödinger operators with δ'-potentials on hypersurfaces

In this section we use quasi boundary triples to define and study the Schrödinger operator $A_{\delta',\beta}$ formally corresponding to the differential expression

$$\mathcal{L}_{\delta',\beta} = -\Delta + V - \beta \langle \delta'_\Sigma, \cdot \rangle \, \delta'_\Sigma,$$

where δ'_Σ is the normal derivative of the δ-distribution supported on Σ.

4.3.1 A quasi boundary triple and its Weyl function

Again it is convenient to define a quasi boundary triple not for $A^*_{\mathrm{i,e}}$ itself, but for the adjoint of a symmetric intermediate extension of $A_{\mathrm{i,e}}$. We define an extension

$$\widehat{A} := A_{\mathrm{free}} \cap A_{\mathrm{N,i,e}} = \mathcal{L} \upharpoonright \bigl\{ f \in H^2(\mathbb{R}^n) \colon \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma = \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma = 0 \bigr\} \tag{4.3.1}$$

of the orthogonal sum $A_{\mathrm{i,e}}$ in (4.1.9) as the underlying symmetric operator for the quasi boundary triple. Furthermore, we define the operator

$$\widehat{T} := T_{\mathrm{i,e}} \upharpoonright \bigl\{ f_{\mathrm{i}} \oplus f_{\mathrm{e}} \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma) \colon \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma + \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_\Sigma = 0 \bigr\}, \tag{4.3.2}$$

and specify the following two boundary mappings from $\operatorname{dom}\widehat{T}$ into $L^2(\Sigma)$

$$\begin{aligned} \widehat{\Gamma}_0 \colon \ \operatorname{dom}\widehat{T} \to L^2(\Sigma), \quad \widehat{\Gamma}_0 f &:= \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_\Sigma \\ \widehat{\Gamma}_1 \colon \ \operatorname{dom}\widehat{T} \to L^2(\Sigma), \quad \widehat{\Gamma}_1 f &:= f_{\mathrm{e}}|_\Sigma - f_{\mathrm{i}}|_\Sigma. \end{aligned} \tag{4.3.3}$$

Note that the mappings $\widehat{\Gamma}_0$, $\widehat{\Gamma}_1$ are well defined because of the properties of the trace mappings (4.1.4).

In the first proposition of this section we prove that $\{L^2(\Sigma), \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$ is a quasi boundary triple for $\widehat{A}^*$ and we show basic properties of this triple.

Proposition 4.8. *Let the operators $A_{\rm N,i,e}$ and $A_{\rm free}$ be as in (4.1.11) and (4.1.12), respectively. Let the operators $\widehat{A}$ and $\widehat{T}$ and the mappings $\widehat{\Gamma}_0$,$\widehat{\Gamma}_1$ be as in (4.3.1), (4.3.2) and (4.2.3), respectively. Then the triple $\widehat{\Pi} = \{L^2(\Sigma), \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$ is a quasi boundary triple for $\widehat{A}^*$. The restrictions of $\widehat{T}$ to the kernels of the boundary mappings are*

$$\widehat{T} \upharpoonright \ker \widehat{\Gamma}_0 = A_{\rm N,i,e} \quad \textit{and} \quad \widehat{T} \upharpoonright \ker \widehat{\Gamma}_1 = A_{\rm free};$$

and the ranges of these mappings are

$$\operatorname{ran} \widehat{\Gamma}_0 = L^2(\Sigma) \quad \textit{and} \quad \operatorname{ran} \widehat{\Gamma}_1 = H^1(\Sigma).$$

Proof. One can see that $\widehat{\Pi}$ is a quasi boundary triple for $\widehat{A}^*$ in a similar way as in the proof of Proposition 4.1. The abstract Green's identity is a consequence of (4.1.8). Basically, the same argumentation as before yields that $\widehat{T} \upharpoonright \ker \widehat{\Gamma}_0 = A_{\rm N,i,e}$, $\widehat{T} \upharpoonright \ker \widehat{\Gamma}_1 = A_{\rm free}$ and that $\operatorname{ran} \widehat{\Gamma}_0 = L^2(\Sigma)$, $\operatorname{ran} \widehat{\Gamma}_1 \subset H^1(\Sigma)$. Further we show surjectivity of $\widehat{\Gamma}_1$ onto $H^1(\Sigma)$. Fix a function $\chi \in C_0^\infty(\mathbb{R}^n)$ as in the proof of Proposition 4.1, i.e. such that $\chi \equiv 1$ on an open neighbourhood of $\overline{\Omega_{\rm i}}$. Let DL be the double-layer potential associated with the hypersurface Σ and the differential expression $-\Delta + 1$; see, e.g. [McL00, Section 6] for the discussion of double-layer potentials. By [McL00, Theorem 6.11, Theorem 6.12 (ii)] for an arbitrary $\varphi \in H^1(\Sigma)$ the function $f := \chi \mathrm{DL}\varphi$ belongs to $\operatorname{dom} \widehat{T}$ and satisfies the condition

$$f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma = \varphi,$$

hence $\widehat{\Gamma}_1 f = \varphi$, and thus $\operatorname{ran} \widehat{\Gamma}_1 = H^1(\Sigma)$.

$\square$

In the next proposition we clarify the basic properties of the γ-field and the Weyl function associated with the quasi boundary triple $\widehat{\Pi}$ from Proposition 4.8.

Proposition 4.9. *Let the self-adjoint operators $A_{\rm N,i,e}$ and $A_{\rm free}$ be as in (4.1.11) and (4.1.12), respectively. Let $\widehat{\Pi}$ be the quasi boundary triple from Proposition 4.8. Let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and the Weyl function associated with the quasi boundary triple $\widehat{\Pi}$ as in Definition 2.10. Let $M_{\rm i}$ and $M_{\rm e}$ be the Weyl functions defined in (4.1.13). Then the following statements hold.*

(i) *The γ-field $\widehat{\gamma}$ is defined for all $\lambda \in \rho(A_{\rm N,i,e})$ and*

$$\widehat{\gamma}(\lambda)\colon L^2(\Sigma) \to L^2(\mathbb{R}^n), \qquad \widehat{\gamma}(\lambda)\varphi = f_\lambda(\varphi),$$

where $f_\lambda(\varphi)$ is the unique solution in $H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma)$ of the problem

$$
\begin{aligned}
-\Delta f + Vf - \lambda f &= 0, \quad \textit{in } \mathbb{R}^n \setminus \Sigma,\\
\partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma = -\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma &= \varphi, \quad \textit{on } \Sigma.
\end{aligned}
$$

(ii) *The Weyl function $\widehat{M}$ is defined for all $\lambda \in \rho(A_{\mathrm{N,i,e}})$ and*

$$
\widehat{M}(\lambda)\colon L^2(\Sigma) \to L^2(\Sigma), \qquad \widehat{M}(\lambda)\varphi = f_{\lambda,\mathrm{e}}(\varphi)|_\Sigma - f_{\lambda,\mathrm{i}}(\varphi)|_\Sigma,
$$

where $f_\lambda(\varphi) = \widehat{\gamma}(\lambda)\varphi$. For all $\lambda \in \rho(A_{\mathrm{N,i,e}})$ ($\lambda \in \rho(A_{\mathrm{N,i,e}}) \cap \rho(A_{\mathrm{free}})$) the operator $\widehat{M}(\lambda)$ maps $L^2(\Sigma)$ into (onto) $H^1(\Sigma)$. The operator $\widehat{M}(\lambda)$ is compact for all $\lambda \in \rho(A_{\mathrm{N,i,e}})$. Moreover, the identity

$$
\widehat{M}(\lambda) = M_\mathrm{i}(\lambda) + M_\mathrm{e}(\lambda) \tag{4.3.4}
$$

holds for all $\lambda \in \rho(A_{\mathrm{N,i,e}})$.

Proof. (i) The mapping properties of the γ-field $\widehat{\gamma}$ follow from (4.3.3), (4.3.2) and Definition 2.10.

(ii) The mapping properties of the Weyl function $\widehat{M}$ follow from (4.3.3), Definition 2.10, Proposition 2.11 (iii) and Proposition 4.8. The compactness of the operator $\widehat{M}(\lambda)$ follows from the compactness of the embedding of $H^1(\Sigma)$ into $L^2(\Sigma)$, cf. Lemma 2.22.

Let us verify the identity (4.3.4). For this let $\lambda \in \rho(A_{\mathrm{N,i,e}})$, so that the operators $M_\mathrm{i}(\lambda)$, $M_\mathrm{e}(\lambda)$ and $\widehat{M}(\lambda)$ all exist. If $\widehat{M}(\lambda)\varphi = \psi$ for some $\varphi \in L^2(\Sigma)$ and $\psi \in H^1(\Sigma)$, then there exists $f = f_\mathrm{i} \oplus f_\mathrm{e} \in \ker(\widehat{T} - \lambda)$ such that

$$
\widehat{\Gamma}_0 f = \varphi \quad \text{and} \quad \widehat{\Gamma}_1 f = \psi.
$$

As $f_\mathrm{i} \in \ker(T_\mathrm{i} - \lambda)$ and $f_\mathrm{e} \in \ker(T_\mathrm{e} - \lambda)$, we have

$$
\begin{aligned}
f_\mathrm{i}|_\Sigma &= M_\mathrm{i}(\lambda)(\partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma) = -M_\mathrm{i}(\lambda)\varphi,\\
f_\mathrm{e}|_\Sigma &= M_\mathrm{e}(\lambda)(\partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma) = M_\mathrm{e}(\lambda)\varphi,
\end{aligned}
$$

and hence

$$
\widehat{M}(\lambda)\varphi = f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma = M_\mathrm{e}(\lambda)\varphi + M_\mathrm{i}(\lambda)\varphi.
$$

Since this is true for arbitrary $\varphi \in L^2(\Sigma)$, relation (4.3.4) follows. □

Remark 4.10. Assume for simplicity that the potential V in the differential expression $\mathcal{L}$ in (4.1.1) is identically equal to zero. Note that the problem in Proposition 4.9 (i) is decoupled into an interior and an exterior problem. Let, as in Remark 4.3, G_λ be the integral kernel of the resolvent of $A_{\rm free}$. Then for all $\psi \in C^\infty(\Sigma)$

$$\big(\widehat{\gamma}(\lambda)\psi\big)(x) = \int_\Sigma \big[\partial_{\nu_{\rm i}(y)} G_\lambda(x,y)\big]\big(\widehat{M}(\lambda)\psi\big)(y)d\sigma_y, \quad x \in \mathbb{R}^n \setminus \Sigma,$$

and

$$\big(\widehat{M}(\lambda)^{-1}\psi\big)(x) = -\partial_{\nu_{\rm i}(x)} \int_\Sigma \big[\partial_{\nu_{\rm i}(y)} G_\lambda(x,y)\big]\psi(y)d\sigma_y, \quad x \in \Sigma,$$

where $\partial_{\nu_{\rm i}(x)}$ and $\partial_{\nu_{\rm i}(y)}$ are the normal derivatives with respect to the first and second arguments with normals pointing outwards of $\Omega_{\rm i}$, and σ_y is the natural Lebesgue measure on Σ. Note that the operator $\widehat{\gamma}(\lambda)$ is, roughly speaking, an extension of the acoustic double-layer potential for the Helmholtz equation multiplied with $\widehat{M}(\lambda)$ and $\widehat{M}(\lambda)^{-1}$ is a hypersingular operator, see, e.g. [McL00, Chapter 6] and [CK83, Co88]. The representation of $\widehat{M}(\lambda)^{-1}$, given above, appears also in [R09] in a slightly different context.

4.3.2 Self-adjointness and Krein's formulae

In the first theorem of this subsection we establish a correspondence between the point spectra of the self-adjoint operator $A_{\rm free}$ and of the operator-valued function $\widehat{M}(\cdot)$. Moreover, we provide a factorization (Krein's formula) for the resolvent difference of $A_{\rm free}$ and $A_{\rm N,i,e}$.

Theorem 4.11. *Let the self-adjoint operators $A_{\rm N,i,e}$ and $A_{\rm free}$ be as in (4.1.11) and (4.1.12), respectively. Let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and the Weyl function from Proposition 4.9. Then the following statements hold.*

(i) *For all $\lambda \in \mathbb{R} \cap \rho(A_{\rm N,i,e})$*

$$\lambda \in \sigma_{\rm p}(A_{\rm free}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\rm p}(\widehat{M}(\lambda))$$

and the multiplicities of these eigenvalues coincide.

(ii) *The formula*

$$(A_{\rm N,i,e} - \lambda)^{-1} - (A_{\rm free} - \lambda)^{-1} = \widehat{\gamma}(\lambda)\widehat{M}(\lambda)^{-1}\widehat{\gamma}(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{\rm N,i,e}) \cap \rho(A_{\rm free})$.

Proof. The equivalence between the point spectra in item (i) and Krein's formula in item (ii) follow from the corresponding items of Theorem 2.13 with self-adjoint $A_0 = A_{\mathrm{N,i,e}}$ ans $A_1 = A_{\mathrm{free}}$. $\square$

We introduce a family of restrictions on the operator $\widehat{T}$ parameterized by a boundedly invertible real-valued function on Σ.

Definition 4.12. For a real-valued function β such that $1/\beta \in L^\infty(\Sigma)$ the Schrödinger operator with δ'-potential on the hypersurface Σ and strength β is defined as follows:

$$A_{\delta',\beta} := \widehat{T} \upharpoonright \ker(\widehat{\Gamma}_1 - \beta\widehat{\Gamma}_0),$$

which is equivalent to

$$\begin{aligned} A_{\delta',\beta} f &= -\Delta f + Vf, \\ \operatorname{dom} A_{\delta',\beta} &= \left\{ f \in H^{3/2}_\Delta(\mathbb{R}^n \setminus \Sigma) \colon \begin{array}{c} \partial_{\nu_\mathrm{i}} f_\mathrm{i}|_\Sigma = -\partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma \\ f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma = \beta \partial_{\nu_\mathrm{e}} f_\mathrm{e}|_\Sigma \end{array} \right\}. \end{aligned} \tag{4.3.5}$$

The definition of $A_{\delta',\beta}$ is compatible with the definition of a point δ'-interaction in the one-dimensional case [AGHH05, Section I.4], [AK00] and the definition of the operator with δ'-potentials on spheres given in [AGS87, Sh88]. Note that, in contrast to the domain of $A_{\delta,\alpha}$, the domain of $A_{\delta',\beta}$ is not contained in $H^1(\mathbb{R}^n)$.

$$\overline{\widehat{T}} = \widehat{A}^* \qquad \overline{T}_{\mathrm{i,e}} = A^*_{\mathrm{i,e}}$$

$$\begin{array}{ccccccccc} & & & & A_{\mathrm{N,i,e}} & & & & \\ & & & \rotatebox{45}{$\subset$} & & \rotatebox{135}{$\subset$} & & & \\ A_{\mathrm{i,e}} & \subset & \widehat{A} & \subset & A_{\delta',\beta} & \subset & \widehat{T} & \subset & T_{\mathrm{i,e}} \\ & & & \rotatebox{-45}{$\subset$} & & \rotatebox{-135}{$\subset$} & & & \\ & & & & A_{\mathrm{free}} & & & & \end{array}$$

Figure 4.2: This figure shows how the operator $A_{\delta',\beta}$ is related to the other operators introduced in this chapter. The operators $A_{\mathrm{N,i,e}}$, $A_{\delta',\beta}$ and A_{free} are self-adjoint in $L^2(\mathbb{R}^n)$, cf. Theorem 4.13.

The next theorem is the counterpart of Theorem 4.6 and can be proved in the same way. Theorem 4.13 shows self-adjointness of $A_{\delta',\beta}$, provides a factorization for the resolvent difference of $A_{\delta',\beta}$ and $A_{\mathrm{N,i,e}}$ via Krein's formula and a variant of the Birman–Schwinger principle.

Theorem 4.13. *Let $A_{\delta',\beta}$ be as above and let $A_{\mathrm{N,i,e}}$ be the self-adjoint operator defined in (4.1.11). Let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and the Weyl function from Proposition 4.9. Then the following statements hold.*

(i) *The operator $A_{\delta',\beta}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R}^n)$.*

(ii) *For all $\lambda \in \mathbb{R} \cap \rho(A_{\mathrm{N,i,e}})$*

$$\lambda \in \sigma_{\mathrm{p}}(A_{\delta',\beta}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}\big(I - \beta^{-1}\widehat{M}(\lambda)\big)$$

and the multiplicities of these eigenvalues coincide.

(iii) *The factorization (Krein's formula)*

$$(A_{\delta',\beta} - \lambda)^{-1} - (A_{\mathrm{N,i,e}} - \lambda)^{-1} = \widehat{\gamma}(\lambda)\big(I - \beta^{-1}\widehat{M}(\lambda)\big)^{-1}\beta^{-1}\,\widehat{\gamma}(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{N,i,e}})$. In this formula the middle term on the right-hand side satisfies $(I - \beta^{-1}\widehat{M}(\lambda))^{-1} \in \mathcal{B}(L^2(\Sigma))$.

Recall that the spaces $H^{3/2}_{\Delta}(\mathbb{R}^n \setminus \Sigma)$ and $H^2(\mathbb{R}^n \setminus \Sigma)$ are defined as in Section 4.1 and the space $W^{1,\infty}(\Sigma)$ is defined as in Section 2.3. It follows from Definition 4.12 that $\operatorname{dom} A_{\delta',\beta} \subset H^{3/2}_{\Delta}(\mathbb{R}^n \setminus \Sigma)$. As in the previous chapter additional smoothness of the coefficient in the boundary condition leads to $\operatorname{dom} A_{\delta',\beta} \subset H^2(\mathbb{R}^n \setminus \Sigma)$. In the next theorem we clarify this property.

Theorem 4.14. *Assume that a real-valued function β is such that $1/\beta \in W^{1,\infty}(\Sigma)$. Let the self-adjoint operator $A_{\delta',\beta}$ be as in Definition 4.12. Then the inclusion $\operatorname{dom} A_{\delta',\beta} \subset H^2(\mathbb{R}^n \setminus \Sigma)$ holds.*

Proof. The proof is analogous to the proof of Theorem 4.7 with $A_{\delta,\alpha}$, A_{free}, $\widetilde{T}$, $\widetilde{\Gamma}_0$, $\widetilde{\Gamma}_1$ and α replaced by $A_{\delta',\beta}$, $A_{\mathrm{N,i,e}}$, $\widehat{T}$, $\widehat{\Gamma}_0$, $\widehat{\Gamma}_1$ and $1/\beta$, respectively. Instead of the decomposition (4.2.8) one can use the decomposition

$$\operatorname{dom} \widehat{T} = \operatorname{dom} A_{\mathrm{N,i,e}} \dotplus \ker(\widehat{T} - \lambda), \qquad \lambda \in \mathbb{C} \setminus \mathbb{R}.$$

$\square$

4.4 Operator ideal properties of resolvent power differences and trace formulae

In this section we obtain $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power differences of the self-adjoint Schrödinger operators with distinct couplings on the hypersurface Σ. As a consequence of these estimates we get sufficient conditions for the existence and completeness of the wave operators for the scattering pairs formed by the free Schrödinger operator $A_{\rm free}$ and one of the Schrödinger operators $A_{\delta,\alpha}$, $A_{\delta',\beta}$, $A_{\rm N,i,e}$ and $A_{\rm D,i,e}$ with certain couplings. In the case of trace class resolvent power difference we provide formulae, where the trace of the resolvent power difference, acting in $\mathbb{R}^n$, is reduced to the trace of a certain operator acting on Σ.

4.4.1 Elliptic regularity and some preliminary $\mathfrak{S}_{p,\infty}$-estimates

In this subsection we first provide a typical regularity result for the functions $(A_{\rm free} - \lambda)^{-1} f$ and $(A_{\rm N,i,e} - \lambda)^{-1} f$ if f and V satisfy some additional local smoothness assumptions. This fact is then used to obtain estimates for the singular values of certain compact operators arising in the representations of the resolvent power differences of the self-adjoint operators $A_{\delta,\alpha}$, $A_{\delta',\beta}$, $A_{\rm free}$, $A_{\rm N,i,e}$ and $A_{\rm D,i,e}$. In the next lemma we make use of the local Sobolev spaces $W^{k,\infty}_\Sigma(\mathbb{R}^n)$, $W^{k,\infty}_\Sigma(\mathbb{R}^n \setminus \Sigma)$ and $H^k_\Sigma(\mathbb{R}^n)$, $H^k_\Sigma(\mathbb{R}^n \setminus \Sigma)$ defined in Section 4.1.

Lemma 4.15. *Let $A_{\rm N,i,e}$ and $A_{\rm free}$ be the self-adjoint operators from and (4.1.11) and (4.1.12), respectively, and let $m \in \mathbb{N}_0$. Then the following assertions hold.*

(i) *If $V \in W^{m,\infty}_\Sigma(\mathbb{R}^n)$, then for all $\lambda \in \rho(A_{\rm free})$ and $k = 0, 1, \dots, m$,*

$$f \in H^k_\Sigma(\mathbb{R}^n) \quad \Longrightarrow \quad (A_{\rm free} - \lambda)^{-1} f \in H^{k+2}_\Sigma(\mathbb{R}^n).$$

(ii) *If $V \in W^{m,\infty}_\Sigma(\mathbb{R}^n \setminus \Sigma)$, then for all $\lambda \in \rho(A_{\rm N,i,e})$ and $k = 0, 1, \dots, m$,*

$$f \in H^k_\Sigma(\mathbb{R}^n \setminus \Sigma) \quad \Longrightarrow \quad (A_{\rm N,i,e} - \lambda)^{-1} f \in H^{k+2}_\Sigma(\mathbb{R}^n \setminus \Sigma).$$

Proof. We verify only assertion (i); the proof of (ii) is similar. We proceed by induction with respect to k. For $k = 0$ the statement is an immediate consequence of $H^0_\Sigma(\mathbb{R}^n) = L^2(\mathbb{R}^n)$ and $\operatorname{dom} A_{\rm free} = H^2(\mathbb{R}^n)$. Suppose now that the implication in (i) is true for some fixed $k < m$ and let $f \in H^{k+1}_\Sigma(\mathbb{R}^n)$. Then, in particular, $f \in H^k_\Sigma(\mathbb{R}^n)$ and hence

$$u := (A_{\rm free} - \lambda)^{-1} f \in H^{k+2}_\Sigma(\mathbb{R}^n) \subset H^{k+1}_\Sigma(\mathbb{R}^n)$$

by assumption. As $k+1 \leq m$ and $V \in W^{m,\infty}_\Sigma(\mathbb{R}^n)$, it follows from (2.3.4) that $Vu \in H^{k+1}_\Sigma(\mathbb{R}^n)$. Therefore $f - Vu \in H^{k+1}_\Sigma(\mathbb{R}^n)$, and since the function u satisfies the partial differential equation

$$-\Delta u - \lambda u = f - Vu, \quad \text{in } \mathbb{R}^n,$$

standard results on elliptic regularity yield that $u \in H^{k+3}_\Sigma(\mathbb{R}^n)$; see, e.g. [McL00, Theorem 4.18]. $\square$

An application of the previous lemma gives the following proposition, in which we provide certain preliminary $\mathfrak{S}_{p,\infty}$-estimates that are useful in the proofs of our main results in the next subsection.

Proposition 4.16. *Let $A_{\mathrm{N,i,e}}$ and A_{free} be the self-adjoint operators from (4.1.11) and (4.1.12), respectively, and let $\widetilde{\gamma}$ and $\widehat{\gamma}$ be the γ-fields from Propositions 4.2 and 4.9, respectively. Then for a fixed $m \in \mathbb{N}_0$ the following statements hold.*

(i) *If $V \in W^{2m,\infty}_\Sigma(\mathbb{R}^n)$, then, for all $\lambda, \mu \in \rho(A_{\mathrm{free}})$ and $k = 0, 1, \dots, m$,*

(a) $\widetilde{\gamma}(\mu)^*(A_{\mathrm{free}} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\mathbb{R}^n), L^2(\Sigma)\big)$,

(b) $\widetilde{\gamma}(\mu)^*(A_{\mathrm{free}} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+1/2},\infty}\big(L^2(\mathbb{R}^n), H^1(\Sigma)\big)$,

(c) $(A_{\mathrm{free}} - \lambda)^{-k}\widetilde{\gamma}(\mu) \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\Sigma), L^2(\mathbb{R}^n)\big)$.

(ii) *If $V \in W^{2m,\infty}_\Sigma(\mathbb{R}^n \backslash \Sigma)$, then, for all $\lambda, \mu \in \rho(A_{\mathrm{N,i,e}})$ and $k = 0, 1, \dots, m$,*

(a) $\widehat{\gamma}(\mu)^*(A_{\mathrm{N,i,e}} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\mathbb{R}^n), L^2(\Sigma)\big)$,

(b) $\widehat{\gamma}(\mu)^*(A_{\mathrm{N,i,e}} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+1/2},\infty}\big(L^2(\mathbb{R}^n), H^1(\Sigma)\big)$,

(c) $(A_{\mathrm{N,i,e}} - \lambda)^{-k}\widehat{\gamma}(\mu) \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\Sigma), L^2(\mathbb{R}^n)\big)$.

Proof. We prove assertion (i); the proof of (ii) is analogous. As

$$\operatorname{ran}(A_{\mathrm{free}} - \lambda)^{-1} = \operatorname{dom} A_{\mathrm{free}} = H^2(\mathbb{R}^n) \subset H^2_\Sigma(\mathbb{R}^n)$$

we conclude from Lemma 4.15 (i) that the inclusion

$$\operatorname{ran}\big((A_{\mathrm{free}} - \overline{\mu})^{-1}(A_{\mathrm{free}} - \lambda)^{-k}\big) \subset H^{2k+2}_\Sigma(\mathbb{R}^n)$$

holds for all $k = 0, 1, \dots, m$. Moreover, since by Proposition 3.1 we have $A_{\mathrm{free}} = \widetilde{T} \upharpoonright \ker \widetilde{\Gamma}_0$, Proposition 2.11 (ii) implies that

$$\widetilde{\gamma}(\mu)^*(A_{\mathrm{free}} - \lambda)^{-k} = \widetilde{\Gamma}_1(A_{\mathrm{free}} - \overline{\mu})^{-1}(A_{\mathrm{free}} - \lambda)^{-k}$$

and hence

$$\operatorname{ran}\bigl(\widetilde{\gamma}(\mu)^*(A_{\mathrm{free}} - \lambda)^{-k}\bigr) \subset H^{2k+3/2}(\Sigma) \tag{4.4.1}$$

by the properties of the trace map $\widetilde{\Gamma}_1$, cf. (4.1.3). Now the estimates in (a) and (b) follow from (4.4.1) and Lemma 2.22 with $\mathcal{K} = L^2(\mathbb{R}^n)$, $r_2 = 2k + \frac{3}{2}$ and with $r_1 = 0$ for (a) and $r_1 = 1$ for (b), respectively. The estimate in (c) follows from (a) by taking the adjoint. Note that in the proof of item (ii) one needs Lemma 4.15 (ii). □

4.4.2 Resolvent power differences in $\mathfrak{S}_{p,\infty}$-classes

In the next two theorems we obtain $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power differences of the self-adjoint free and decoupled Schrödinger operators A_{free} and $A_{\mathrm{N,i,e}}$, $A_{\mathrm{D,i,e}}$ with certain local smoothness assumptions on the potential V in the differential expression.

Theorem 4.17. *Let $A_{\mathrm{D,i,e}}$ and A_{free} be the self-adjoint operators defined in (4.1.10) and (4.1.12), respectively. Let $\widetilde{M}$ be the Weyl function from Proposition 4.2. Assume that for some $m \in \mathbb{N}$ the potential V satisfies $V \in W^{2m-2,\infty}_{\Sigma}(\mathbb{R}^n)$. Then the following statements hold.*

(i) *For all $l = 1, 2, \dots, m$ and all $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{N,i,e}})$*

$$(A_{\mathrm{free}} - \lambda)^{-l} - (A_{\mathrm{D,i,e}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\bigl(L^2(\mathbb{R}^n)\bigr). \tag{4.4.2}$$

(ii) *If $m > \frac{n-1}{2}$, then for all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \leq m$, and all $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{D,i,e}})$ the resolvent power difference in (4.4.2) belongs to the trace class, and the formula*

$$\begin{aligned} &\operatorname{tr}\bigl((A_{\mathrm{free}} - \lambda)^{-l} - (A_{\mathrm{D,i,e}} - \lambda)^{-l}\bigr) \\ &\qquad = \frac{1}{(l-1)!}\operatorname{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Bigl(\widetilde{M}(\lambda)^{-1}\widetilde{M}'(\lambda)\Bigr)\right) \end{aligned} \tag{4.4.3}$$

holds.

Proof. (i) Fix an arbitrary $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and let $\widetilde{\gamma}$ be the γ-field as in Proposition 4.2. By Theorem 4.4 (ii) the resolvent difference of A_{free} and $A_{\mathrm{D,i,e}}$ at the point λ_0 can be written in the form

$$(A_{\mathrm{free}} - \lambda_0)^{-1} - (A_{\mathrm{D,i,e}} - \lambda_0)^{-1} = \widetilde{\gamma}(\lambda_0)\widetilde{M}(\lambda_0)^{-1}\widetilde{\gamma}(\overline{\lambda}_0)^*.$$

Furthermore, by Proposition 4.2 (ii) the operator $\widetilde{M}(\lambda_0)$ is bijective and closed as an operator from $L^2(\Sigma)$ onto $H^1(\Sigma)$. Hence, $\mathrm{dom}\,\big(\widetilde{M}(\lambda_0)^{-1}\big) = H^1(\Sigma)$ and since, $\widetilde{M}(\lambda_0)^{-1}$ is closed as an operator from $H^1(\Sigma)$ into $L^2(\Sigma)$, we conclude that $\widetilde{M}(\lambda_0)^{-1} \in \mathcal{B}\big(H^1(\Sigma), L^2(\Sigma)\big)$. Set

$$H := A_{\mathrm{D,i,e}}, \quad K := A_{\mathrm{free}}, \quad F_1 := \widetilde{\gamma}(\lambda_0), \quad F_2 := M(\lambda_0)^{-1}\widetilde{\gamma}(\overline{\lambda}_0)^*.$$

Then Proposition 4.16 (i) implies that the assumptions in Lemma 2.4 are satisfied with

$$a = \frac{2}{n-1}, \quad b_1 = \frac{3/2}{n-1}, \quad b_2 = \frac{1/2}{n-1}, \quad r = m.$$

Since $b = b_1 + b_2 - a = 0$, Lemma 2.4 implies

$$(A_{\mathrm{free}} - \lambda)^{-l} - (A_{\mathrm{D,i,e}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big)$$

for all $\lambda \in \rho(A_{\mathrm{N,i,e}}) \cap \rho(A_{\mathrm{free}})$.

(ii) For all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \le m$, the operator in (4.4.2) belongs to the trace class by item (i). The trace formula can be proved as in Theorem 3.12 (ii) with A_{D}, A_{N}, M and γ replaced by $A_{\mathrm{D,i,e}}$, A_{free}, $\widetilde{M}$ and $\widetilde{\gamma}$, respectively. ☐

Theorem 4.18. *Let $A_{\mathrm{N,i,e}}$ and A_{free} be the self-adjoint operators defined in (4.1.11) and (4.1.12), respectively. Let $\widehat{M}$ be the Weyl function from Proposition 4.9. Assume that for some $m \in \mathbb{N}$ the potential V satisfies $V \in W^{2m-2,\infty}_{\Sigma}(\mathbb{R}^n \setminus \Sigma)$. Then the following statements hold.*

(i) *For all $l = 1, 2, \ldots, m$ and all $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{N,i,e}})$*

$$(A_{\mathrm{N,i,e}} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.4}$$

(ii) *If $m > \frac{n-1}{2}$, then for all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \le m$, and all $\lambda \in \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{N,i,e}})$ the resolvent power difference in (4.4.4) belongs to the trace class, and the formula*

$$\begin{aligned}&\mathrm{tr}\,\big((A_{\mathrm{N,i,e}} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l}\big)\\ &\qquad = \frac{1}{(l-1)!}\,\mathrm{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Big(\widehat{M}(\lambda)^{-1}\widehat{M}'(\lambda)\Big)\right)\end{aligned} \tag{4.4.5}$$

holds.

Proof. (i) We fix an arbitrary $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and let $\widehat{\gamma}$ be the γ-field from Proposition 4.9. By Theorem 4.11 (ii) the resolvent difference of A_{free} and $A_{\mathrm{N,i,e}}$ at the point λ_0 can be written in the form

$$(A_{\mathrm{N,i,e}} - \lambda_0)^{-1} - (A_{\mathrm{free}} - \lambda_0)^{-1} = \widehat{\gamma}(\lambda_0)\widehat{M}(\lambda_0)^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*.$$

Furthermore, by Proposition 4.9 (ii) the operator $\widehat{M}(\lambda_0)$ is bijective and closed as an operator from $L^2(\Sigma)$ onto $H^1(\Sigma)$. Hence, $\mathrm{dom}\big(\widehat{M}(\lambda_0)^{-1}\big) = H^1(\Sigma)$ and since, $\widehat{M}(\lambda_0)^{-1}$ is closed as an operator from $H^1(\Sigma)$ into $L^2(\Sigma)$, we conclude $\widehat{M}(\lambda_0)^{-1} \in \mathcal{B}\big(H^1(\Sigma), L^2(\Sigma)\big)$. Set

$$H := A_{\mathrm{free}}, \quad K := A_{\mathrm{N,i,e}}, \quad F_1 := \widehat{\gamma}(\lambda_0), \quad F_2 := \widehat{M}(\lambda_0)^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*.$$

Then Proposition 4.16 (ii) (b) and (c) imply that the assumptions in Lemma 2.4 are satisfied with

$$a = \frac{2}{n-1}, \quad b_1 = \frac{3/2}{n-1}, \quad b_2 = \frac{1/2}{n-1}, \quad r = m.$$

Since $b = b_1 + b_2 - a = 0$, Lemma 2.4 implies

$$(A_{\mathrm{N,i,e}} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big)$$

for all $\lambda \in \rho(A_{\mathrm{N,i,e}}) \cap \rho(A_{\mathrm{free}})$.

(ii) For all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \leq m$, the operator in (4.4.4) belongs to the trace class by item (i). The trace formula can be proved as in Theorem 3.12 (ii) with A_{D}, A_{N}, M and γ replaced by A_{free}, $A_{\mathrm{N,i,e}}$, $\widehat{M}$ and $\widehat{\gamma}$, respectively. $\square$

As a consequence of Theorems 4.17 and 4.18 we derive sufficient condition for the existence and completeness of the wave operators of the scattering pairs $\{A_{\mathrm{free}}, A_{\mathrm{D,i,e}}\}$ and $\{A_{\mathrm{free}}, A_{\mathrm{N,i,e}}\}$.

Corollary 4.19. *Let $A_{\mathrm{D,i,e}}$, $A_{\mathrm{N,i,e}}$ and A_{free} be the self-adjoint operators defined in (4.1.10),(4.1.11) and (4.1.12), respectively. Assume that the potential V satisfies $V \in W^{k,\infty}_{\Sigma}(\mathbb{R}^n)$ with $k > n-3$. Then the following statements hold.*

(i) *The wave operators $W_{\pm}(A_{\mathrm{free}}, A_{\mathrm{D,i,e}})$ for the scattering pair $\{A_{\mathrm{free}}, A_{\mathrm{D,i,e}}\}$ exist and are complete, and hence the absolutely continuous parts of $A_{\mathrm{D,i,e}}$ and A_{free} are unitarily equivalent.*

(ii) *The wave operators $W_\pm(A_{\mathrm{free}}, A_{\mathrm{N,i,e}})$ for the scattering pair $\{A_{\mathrm{free}}, A_{\mathrm{N,i,e}}\}$ exist and are complete, and hence the absolutely continuous parts of $A_{\mathrm{N,i,e}}$ and A_{free} are unitarily equivalent.*

Remark 4.20. In particular, if $V \equiv 0$, then the wave operators for the scattering pairs $\{A_{\mathrm{free}}, A_{\mathrm{D,i,e}}\}$ and $\{A_{\mathrm{free}}, A_{\mathrm{N,i,e}}\}$ exist and are complete for all space dimensions $n \geq 2$ and $\sigma_{\mathrm{ac}}(A_{\mathrm{D,e}}) = \sigma_{\mathrm{ac}}(A_{\mathrm{N,e}}) = \big[0, \infty\big)$.

Remark 4.21. Note that for the pair $\{A_{\mathrm{free}}, A_{\mathrm{N,i,e}}\}$ the assumption in Corollary 4.19 on the smoothness of the potential V can be slightly weakened, cf. Theorem 4.18.

In the next theorem we obtain $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power difference of the self-adjoint operators $A_{\delta,\alpha}$ and A_{free}. One can observe that the singular values may converge faster than in Theorems 4.17 and 4.18.

Theorem 4.22. *Let $\alpha \in L^\infty(\Sigma)$ be a real-valued function on Σ, and let $A_{\delta,\alpha}$ and A_{free} be the self-adjoint operators defined in (4.2.6) and (4.1.12), respectively. Let $\widetilde{M}$ be the Weyl function from Proposition 4.2. Assume that the potential V satisfies $V \in W^{2m-2,\infty}_\Sigma(\mathbb{R}^n)$ for some $m \in \mathbb{N}$. Then the following statements hold.*

(i) *For all $l = 1, 2, \dots, m$ and all $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\mathrm{free}})$*

$$(A_{\delta,\alpha} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.6}$$

(ii) *If $m > \frac{n}{2} - 1$, then for all $l \in \mathbb{N}$ such that $\frac{n}{2} - 1 < l \leq m$, the resolvent power difference in (4.4.6) belongs to the trace class, and the formula*

$$\begin{aligned}\operatorname{tr}\big((A_{\delta,\alpha} - \lambda)^{-l} &- (A_{\mathrm{free}} - \lambda)^{-l}\big)\\ &= \frac{1}{(l-1)!}\operatorname{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Big(\widetilde{U}(\lambda)\widetilde{M}'(\lambda)\Big)\right)\end{aligned}$$

holds, where $\widetilde{U}(\lambda) := \big(I - \alpha\widetilde{M}(\lambda)\big)^{-1}\alpha$.

Proof. (i) We prove item (i) by applying Lemma 2.4. Fix an arbitrary $\lambda_0 \in \mathbb{C}\setminus\mathbb{R}$, and let $\widetilde{\gamma}$ be as in Proposition 4.2. By Theorem 4.6 the resolvent difference of $A_{\delta,\alpha}$ and A_{free} at the point λ_0 can be written in the form

$$(A_{\delta,\alpha} - \lambda_0)^{-1} - (A_{\mathrm{free}} - \lambda_0)^{-1} = \widetilde{\gamma}(\lambda_0)\big(I - \alpha\widetilde{M}(\lambda_0)\big)^{-1}\alpha\widetilde{\gamma}(\overline{\lambda}_0)^*,$$

where $(I-\alpha\widetilde{M}(\lambda_0))^{-1}\alpha \in \mathcal{B}(L^2(\Sigma))$. Proposition 4.16 (i) (a) and (c) imply that the assumptions in Lemma 2.4 are satisfied with

$$\begin{aligned} &H = A_{\delta,\alpha}, \quad K = A_{\text{free}}, \quad F_1 = \widetilde{\gamma}(\lambda_0), \quad F_2 = \big(I-\alpha\widetilde{M}(\lambda_0)\big)^{-1}\alpha\widetilde{\gamma}(\overline{\lambda}_0)^*, \\ &a = \frac{2}{n-1}, \quad b_1 = b_2 = \frac{3/2}{n-1}, \quad r = m. \end{aligned}$$

Since $b = b_1 + b_2 - a = \frac{1}{n-1}$, Lemma 2.4 implies the assertion of the theorem.

(ii) By item (i) the operator in (4.4.6) belongs to the trace class for all $l \in \mathbb{N}$ such that $\frac{n}{2} - 1 < l \le m$. The trace formula can be proved as in Theorem 3.17 (ii) with $A_{[B_1]}$, $A_{[B_2]}$, M, γ, B_1 and B_2 replaced by $A_{\delta,\alpha}$, A_{free}, $\widetilde{M}$, $\widetilde{\gamma}$, α and 0, respectively. $\square$

The next corollary shows that for sufficiently smooth potentials V the wave operators of the scattering system $\{A_{\delta,\alpha}, A_{\text{free}}\}$ exist in any space dimension.

Corollary 4.23. *Let the assumptions be as in Theorem 4.22. If, for some $k > n-4$, the potential V satisfies $V \in W^{k,\infty}_{\Sigma}(\mathbb{R}^n)$, then the wave operators $W_\pm(A_{\delta,\alpha}, A_{\text{free}})$ exist and are complete, and hence the absolutely continuous parts of $A_{\delta,\alpha}$ and A_{free} are unitarily equivalent.*

Remark 4.24. In particular, if $V \equiv 0$, then $W_\pm(A_{\delta,\alpha}, A_{\text{free}})$ exist and are complete in any space dimension $n \ge 2$. Furthermore, we obtain that $\sigma_{\text{ac}}(A_{\delta,\alpha}) = [0,\infty)$.

In the next theorem we obtain $\mathfrak{S}_{p,\infty}$-estimates for the resolvent power differences of the self-adjoint operators $A_{\delta',\beta}$ and $A_{\text{N,i,e}}$. One can notice the same faster convergence of the singular values as in Theorem 4.22.

Theorem 4.25. *Let β be a real-valued function on Σ such that $1/\beta \in L^\infty(\Sigma)$, and let $A_{\delta',\beta}$ and $A_{\text{N,i,e}}$ be the self-adjoint operators defined in (4.3.5) and (4.1.11), respectively. Let $\widehat{M}$ be the Weyl function from Proposition 4.9. Assume that the potential V satisfies $V \in W^{2m-2,\infty}_{\Sigma}(\mathbb{R}^n \backslash \Sigma)$ for some $m \in \mathbb{N}$. Then the following statements hold.*

(i) *For all $l = 1, 2, \ldots, m$ and all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{free}})$*

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\text{N,i,e}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.7}$$

(ii) *If $m > \frac{n}{2} - 1$, then for all $l \in \mathbb{N}$ such that $\frac{n}{2} - 1 < l \leq m$, the resolvent power difference in (4.4.7) belongs to the trace class, and the formula*

$$\operatorname{tr}\big((A_{\delta',\beta} - \lambda)^{-l} - (A_{\mathrm{N,i,e}} - \lambda)^{-l}\big) = \frac{1}{(l-1)!} \operatorname{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Big(\widehat{U}(\lambda)\widehat{M}'(\lambda)\Big)\right)$$

holds, where $\widehat{U}(\lambda) := \big(I - \beta^{-1}\widehat{M}(\lambda)\big)^{-1}\beta^{-1}$.

Proof. (i) Fix an arbitrary $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ and let $\widehat{\gamma}$ be the γ-field from Proposition 4.9. By Theorem 4.13 the resolvent difference of $A_{\delta',\beta}$ and $A_{\mathrm{N,i,e}}$ at the point λ_0 can be written in the form

$$(A_{\delta',\beta} - \lambda_0)^{-1} - (A_{\mathrm{N,i,e}} - \lambda_0)^{-1} = \widehat{\gamma}(\lambda_0)\big(I - \beta^{-1}\widehat{M}(\lambda_0)\big)^{-1}\beta^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*,$$

where $(I - \beta^{-1}\widehat{M}(\lambda_0))^{-1}\beta^{-1} \in \mathcal{B}(L^2(\Sigma))$. Proposition 4.16 (i) (a) and (c) imply that the assumptions in Lemma 2.4 are satisfied with

$$H = A_{\delta',\beta}, \quad K = A_{\mathrm{free}}, \quad F_1 = \widehat{\gamma}(\lambda_0), \quad F_2 = \big(I - \beta^{-1}\widehat{M}(\lambda_0)\big)^{-1}\beta^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*,$$
$$a = \frac{2}{n-1}, \quad b_1 = b_2 = \frac{3/2}{n-1}, \quad r = m.$$

Since $b = b_1 + b_2 - a = \frac{1}{n-1}$, Lemma 2.4 implies the assertion of the theorem.

(ii) By item (i) the operator in (4.4.7) belongs to the trace class for all $l \in \mathbb{N}$ such that $\frac{n}{2} - 1 < l \leq m$. The trace formula can be proved as in Theorem 3.17 (ii) with $A_{[B_2]}$, $A_{[B_1]}$, M, γ, B_2 and B_1 replaced by $A_{\delta',\beta}$, $A_{\mathrm{N,i,e}}$, $\widehat{M}$, $\widehat{\gamma}$, $1/\beta$ and 0, respectively. □

In next theorem we get $\mathfrak{S}_{p,\infty}$-properties of the resolvent power difference of $A_{\delta',\beta}$ and A_{free}.

Theorem 4.26. *Let β be a real-valued function on Σ such that $1/\beta \in L^\infty(\Sigma)$, and let $A_{\delta',\beta}$, $A_{\mathrm{N,i,e}}$ and A_{free} be the self-adjoint operators defined in (4.3.5), (4.1.11) and (4.1.12), respectively. Let $\widehat{M}$ be the Weyl function from Proposition 4.9. Assume that the potential V satisfies $V \in W^{2m-2,\infty}_\Sigma(\mathbb{R}^n \setminus \Sigma)$ for some $m \in \mathbb{N}$. Then the following statements hold.*

(i) *For all $l = 1, 2, \ldots, m$ and all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{free}})$*

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.8}$$

(ii) *If $m > \frac{n-1}{2}$, then, for all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \leq m$, the resolvent power difference in (4.4.8) belongs to the trace class, and the formula*

$$\begin{aligned}\operatorname{tr}\big((A_{\delta',\beta} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l}\big) \\ = \frac{1}{(l-1)!}\operatorname{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Big(\widehat{V}(\lambda)\widehat{M}'(\lambda)\Big)\right)\end{aligned}$$

holds, where $\widehat{V}(\lambda) := \big(I - \widehat{M}(\lambda)\beta^{-1}\big)^{-1}\widehat{M}(\lambda)^{-1}$.

Proof. (i) Let us fix $\lambda_0 \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{N,i,e}})$. By Theorem 4.18 (i)

$$(A_{\mathrm{free}} - \lambda_0)^{-l} - (A_{\mathrm{N,i,e}} - \lambda_0)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.9}$$

By Theorem 4.25 (i)

$$(A_{\delta',\beta} - \lambda_0)^{-l} - (A_{\mathrm{N,i,e}} - \lambda_0)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n)\big). \tag{4.4.10}$$

Taking the difference of (4.4.9) and (4.4.10) we get the claim for all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{free}}) \cap \rho(A_{\mathrm{N,i,e}})$. In order to include the points in the discrete set $\rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{free}}) \cap \sigma(A_{\mathrm{N,i,e}})$ we argue with contour integrals.

(ii) By item (i) the operator in (4.4.8) belongs to the trace class for all $l \in \mathbb{N}$ such that $\frac{n-1}{2} < l \leq m$. The trace formula can be proved as in Corollary 3.19 (ii) with $A_{[B]}$, A_{D}, A_{N}, M and B replaced by $A_{\delta',\beta}$, A_{free}, $A_{\mathrm{N,i,e}}$, $\widehat{M}$ and β^{-1}, respectively. □

The following corollary is the counterpart of Corollary 4.23 for the scattering system $\{A_{\delta',\beta}, A_{\mathrm{free}}\}$.

Corollary 4.27. *Let the assumptions be as in Theorem 4.25. If the potential V satisfies $V \in W^{k,\infty}_{\Sigma}(\mathbb{R}^n \setminus \Sigma)$ with $k > n-3$, then the wave operators $W_{\pm}(A_{\delta',\beta}, A_{\mathrm{free}})$ exist and are complete, and hence the absolutely continuous parts of $A_{\delta',\beta}$ and A_{free} are unitarily equivalent.*

Remark 4.28. In particular, if $V \equiv 0$, then $W_{\pm}(A_{\delta',\beta}, A_{\mathrm{free}})$ exist and are complete in any space dimension $n \geq 2$. Furthermore, we obtain that $\sigma_{\mathrm{ac}}(A_{\delta',\beta}) = [0,\infty)$.

Remark 4.29. In Chapter 3 trace formulae were proven for C^∞-smooth coefficients, whereas in this chapter we formulate trace formulae for rough potentials and say that the proof is analogous. In the complete proofs of Theorem 4.17 (ii), Theorem 4.18 (ii), Theorem 4.22 (ii), Theorem 4.25 (ii) and Theorem 4.26 (ii) one should tackle the smoothness of the potential V carefully, using Lemma 4.15.

4.5 Sesquilinear forms approach

Another rigorous way to define self-adjoint Schrödinger operators with surface interactions uses closed semi-bounded sesquilinear forms and the first representation theorem. We show below that both approaches lead to the same operators. The sesquilinear form in the δ-case is well-known, see e.g. [BEKS94], while the form in the δ'-case is new to the best of the author's knowledge.

Throughout this section we always assume that $V \equiv 0$ and we write $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ instead of $A_{\delta,\alpha}$ and $A_{\delta',\beta}$, respectively. Using sesquilinear forms we also prove finiteness of the negative spectra of $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$.

4.5.1 Definitions via sesquilinear forms

In the first proposition of this subsection we provide a closed semi-bounded sesquilinear form such that the self-adjoint operator $-\Delta_{\delta,\alpha}$ corresponds to this form by the first representation theorem.

Proposition 4.30. *The sesquilinear form*

$$\mathfrak{t}_{\delta,\alpha}[f,g] := \big(\nabla f, \nabla g\big) - \big(\alpha f|_\Sigma, g|_\Sigma\big)_\Sigma$$

defined for $f, g \in H^1(\mathbb{R}^n)$ is symmetric, closed and semi-bounded from below. The self-adjoint operator corresponding to $\mathfrak{t}_{\delta,\alpha}$ is $-\Delta_{\delta,\alpha}$, i.e.,

$$(-\Delta_{\delta,\alpha} f, g) = \mathfrak{t}_{\delta,\alpha}[f,g]$$

holds for all $f \in \operatorname{dom}(-\Delta_{\delta,\alpha})$ and $g \in H^1(\mathbb{R}^n)$.

Proof. Since α is a real-valued function, it follows that the form $\mathfrak{t}_{\delta,\alpha}$ is symmetric. In order to show that this form is closed and semi-bounded, we consider the forms

$$\mathfrak{t}[f,g] := (\nabla f, \nabla g) \quad \text{and} \quad \mathfrak{t}'[f,g] := -\big(\alpha f|_\Sigma, g|_\Sigma\big)_\Sigma$$

on $H^1(\mathbb{R}^n)$, so that $\mathfrak{t}_{\delta,\alpha} = \mathfrak{t} + \mathfrak{t}'$ holds. Note that $\mathfrak{t}$ is closed and non-negative. Let $t \in (\frac{1}{2}, 1)$ be fixed. Since the trace map is continuous, there exists $c_t > 0$ such that $\|f|_\Sigma\|_{H^{t-1/2}(\Sigma)} \leq c_t \|f_{\rm i}\|_{H^t(\Omega_{\rm i})}$ is valid for all $f = f_{\rm i} \oplus f_{\rm e} \in H^t(\mathbb{R}^n)$. Hence it follows from Ehrling's lemma that for every $\varepsilon > 0$ there exists a constant $C_{\rm i}(\varepsilon)$ such that

$$\|f|_\Sigma\|_\Sigma \leq c_t \|f_{\rm i}\|_{H^t(\Omega_{\rm i})} \leq \varepsilon \|f_{\rm i}\|_{H^1(\Omega_{\rm i})} + C_{\rm i}(\varepsilon)\|f_{\rm i}\|_{L^2(\Omega_{\rm i})} \tag{4.5.1}$$

holds for all $f = f_{\rm i} \oplus f_{\rm e} \in H^1(\mathbb{R}^n)$. Since $\|f\|_{H^1(\mathbb{R}^n)} \geq \|f_{\rm i}\|_{H^1(\Omega_{\rm i})}$ and $\|f\|_{L^2(\mathbb{R}^n)} \geq \|f_{\rm i}\|_{L^2(\Omega_{\rm i})}$, the estimate (4.5.1) implies

$$\|f|_\Sigma\|_\Sigma \leq \varepsilon \|f\|_{H^1(\mathbb{R}^n)} + C_{\rm i}(\varepsilon)\|f\|_{L^2(\mathbb{R}^n)} \tag{4.5.2}$$

The estimate (4.5.2) yields that the form $\mathfrak{t}'$ is bounded with respect to $\mathfrak{t}$ with form bound < 1, and hence $\mathfrak{t}_{\delta,\alpha} = \mathfrak{t} + \mathfrak{t}'$ is closed and semi-bounded by [K95, Theorem VI.1.33]. Thus by the first representation theorem [K95, Theorem VI.2.1] the self-adjoint operator $-\widetilde{\Delta}_{\delta,\alpha}$ corresponds to the form $\mathfrak{t}_{\delta,\alpha}$.

It remains to show that $-\widetilde{\Delta}_{\delta,\alpha} = -\Delta_{\delta,\alpha}$. First we show the inclusion $\mathrm{dom}(-\Delta_{\delta,\alpha}) \subset \mathrm{dom}\,\mathfrak{t}_{\delta,\alpha}$. For this let $f = f_{\rm i} \oplus f_{\rm e} \in \mathrm{dom}(-\Delta_{\delta,\alpha})$. According to (4.2.6) we have, in particular,

$$f_{\rm i} \in H^{3/2}(\Omega_{\rm i}) \subset H^1(\Omega_{\rm i}), \quad f_{\rm e} \in H^{3/2}(\Omega_{\rm e}) \subset H^1(\Omega_{\rm e}), \quad \text{and} \quad f_{\rm i}|_\Sigma = f_{\rm e}|_\Sigma.$$

Making use of [AF03, Theorems 5.24 and 5.29] a standard extension argument implies that $f \in H^1(\mathbb{R}^n)$ and hence $\mathrm{dom}(-\Delta_{\delta,\alpha}) \subset \mathrm{dom}\,\mathfrak{t}_{\delta,\alpha}$.

Next let $f = f_{\rm i} \oplus f_{\rm e} \in \mathrm{dom}(-\Delta_{\delta,\alpha})$ and $g = g_{\rm i} \oplus g_{\rm e} \in \mathrm{dom}\,\mathfrak{t}_{\delta,\alpha}$. Then $\mathfrak{t}_{\delta,\alpha}[f,g]$ is well defined. By the first Green's identity (4.1.7) we have

$$\begin{aligned}(\nabla f_{\rm i}, \nabla f_{\rm i})_{\rm i} - (\partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma, g_{\rm i}|_\Sigma)_\Sigma &= (-\Delta f_{\rm i}, g_{\rm i})_{\rm i},\\ (\nabla f_{\rm e}, \nabla g_{\rm e})_{\rm e} - (\partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma, g_{\rm e}|_\Sigma)_\Sigma &= (-\Delta f_{\rm e}, g_{\rm e})_{\rm e}.\end{aligned}$$

Using this and the relation $\alpha f|_\Sigma = \partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma + \partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma$ we obtain

$$\begin{aligned}\mathfrak{t}_{\delta,\alpha}[f,g] &= (\nabla f, \nabla g) - \big(\alpha f|_\Sigma, g|_\Sigma\big)_\Sigma\\ &= (\nabla f_{\rm i}, \nabla g_{\rm i})_{\rm i} + (\nabla f_{\rm e}, \nabla g_{\rm e})_{\rm e} - \big(\partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma, g_{\rm i}|_\Sigma\big)_\Sigma - \big(\partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma, g_{\rm e}|_\Sigma\big)_\Sigma\\ &= (-\Delta f_{\rm i}, g_{\rm i})_{\rm i} + (-\Delta f_{\rm e}, g_{\rm e})_{\rm e} = \big(-\Delta f, g\big).\end{aligned}$$

Now the first representation theorem (see [K95, Theorem VI.2.1]) implies that $f \in \mathrm{dom}(-\widetilde{\Delta}_{\delta,\alpha})$ and $-\widetilde{\Delta}_{\delta,\alpha} f = -\Delta f$; thus $-\Delta_{\delta,\alpha} \subset -\widetilde{\Delta}_{\delta,\alpha}$. Since both operators $-\Delta_{\delta,\alpha}$ and $-\widetilde{\Delta}_{\delta,\alpha}$ are self-adjoint, we conclude that $-\Delta_{\delta,\alpha} = -\widetilde{\Delta}_{\delta,\alpha}$.

□

In the second proposition of this subsection we provide a symmetric closed semi-bounded sesquilinear form such that the self-adjoint operator $-\Delta_{\delta',\beta}$ corresponds to this form by the first representation theorem.

Proposition 4.31. *The sesquilinear form*

$$\mathfrak{t}_{\delta',\beta}[f,g] := \big(\nabla f, \nabla g\big) - \big(\beta^{-1}(f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma), g_\mathrm{e}|_\Sigma - g_\mathrm{i}|_\Sigma\big)_\Sigma$$

defined for $f, g \in H^1(\mathbb{R}^n \setminus \Sigma)$ is symmetric, closed and semi-bounded from below. The self-adjoint operator corresponding to $\mathfrak{t}_{\delta',\beta}$ is $-\Delta_{\delta',\beta}$, i.e.,

$$(-\Delta_{\delta',\beta} f, g) = \mathfrak{t}_{\delta',\beta}[f,g]$$

holds for all $f \in \mathrm{dom}(-\Delta_{\delta',\beta})$ and $g \in H^1(\mathbb{R}^n \setminus \Sigma)$.

Proof. Since β is a real-valued function, it follows that the form $\mathfrak{t}_{\delta',\beta}$ is symmetric. In order to show that it is closed and semi-bounded, we consider the forms

$$\mathfrak{t}[f,g] := (\nabla f, \nabla g) \quad \text{and} \quad \mathfrak{t}'[f,g] := -\big(\beta^{-1}(f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma), g_\mathrm{e}|_\Sigma - g_\mathrm{i}|_\Sigma\big)_\Sigma$$

on $H^1(\mathbb{R}^n \setminus \Sigma)$, so that $\mathfrak{t}_{\delta',\beta} = \mathfrak{t} + \mathfrak{t}'$ holds. Note that $\mathfrak{t}$ is closed and non-negative. Let $t \in (\frac{1}{2}, 1)$ be fixed. Since the trace map is continuous, there exists $c_t > 0$ such that $\|f_\mathrm{i}|_\Sigma\|_{H^{t-1/2}(\Sigma)} \le c_t \|f_\mathrm{i}\|_{H^t(\Omega_\mathrm{i})}$ is valid for all $f_\mathrm{i} \in H^t(\Omega_\mathrm{i})$. Hence it follows from Ehrling's lemma that for every $\varepsilon > 0$ there exists a constant $C_\mathrm{i}(\varepsilon)$ such that

$$\|f_\mathrm{i}|_\Sigma\|_\Sigma \le c_t \|f_\mathrm{i}\|_{H^t(\Omega_\mathrm{i})} \le \varepsilon \|f_\mathrm{i}\|_{H^1(\Omega_\mathrm{i})} + C_\mathrm{i}(\varepsilon)\|f_\mathrm{i}\|_{L^2(\Omega_\mathrm{i})} \tag{4.5.3}$$

holds for all $f_\mathrm{i} \in H^1(\Omega_\mathrm{i})$. We decompose the exterior domain in the form $\Omega_\mathrm{e} = \Omega_{\mathrm{e},1} \cup \overline{\Omega}_{\mathrm{e},2}$, where $\Omega_{\mathrm{e},1}$ is bounded, $\Omega_{\mathrm{e},2}$ is unbounded, and the C^∞-boundary of $\Omega_{\mathrm{e},1}$ is the disjoint union of Σ and $\partial\Omega_{\mathrm{e},2}$. The restriction of a function f_e to $\Omega_{\mathrm{e},1}$ is denoted by $f_{\mathrm{e},1}$. Then again the continuity of the trace map and Ehrling's lemma show that for every $\varepsilon > 0$ there exists a constant $C_\mathrm{e}(\varepsilon)$ such that

$$\begin{aligned} \|f_\mathrm{e}|_\Sigma\|_\Sigma = \|f_{\mathrm{e},1}|_\Sigma\|_\Sigma &\le \|f_{\mathrm{e},1}|_{\partial\Omega_{\mathrm{e},1}}\|_{L^2(\partial\Omega_{\mathrm{e},1})} \\ &\le \varepsilon \|f_{\mathrm{e},1}\|_{H^1(\Omega_{\mathrm{e},1})} + C_\mathrm{e}(\varepsilon)\|f_{\mathrm{e},1}\|_{L^2(\Omega_{\mathrm{e},1})} \\ &\le \varepsilon \|f_\mathrm{e}\|_{H^1(\Omega_\mathrm{e})} + C_\mathrm{e}(\varepsilon)\|f_\mathrm{e}\|_{L^2(\Omega_\mathrm{e})} \end{aligned} \tag{4.5.4}$$

holds for all $f_\mathrm{e} \in H^1(\Omega_\mathrm{e})$. The estimates (4.5.3) and (4.5.4) yield that the form $\mathfrak{t}'$ is bounded with respect to $\mathfrak{t}$ with form bound < 1, and hence $\mathfrak{t}_{\delta',\beta} = \mathfrak{t} + \mathfrak{t}'$ is closed and semi-bounded by [K95, Theorem VI.1.33]. The remaining statement follows from [K95, Theorem VI.2.1] and similar arguments as in the proof of Proposition 4.30. □

4.5.2 Finiteness of negative spectra

In this subsection we show that the negative spectra of the self-adjoint operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ are finite. We recall some preparatory facts on semi-bounded quadratic forms first.

Definition 4.32. For a (not necessarily closed or semi-bounded) quadratic form $\mathfrak{q}$ in a Hilbert space $\mathcal{H}$ we define the *number of negative squares* $\kappa_-(\mathfrak{q})$ by

$$\kappa_-(\mathfrak{q}) := \sup\Big\{ \dim F \colon F \text{ linear subspace of } \operatorname{dom}\mathfrak{q}\ , \\ \text{such that } \forall\, f \in F \setminus \{0\} \colon \mathfrak{q}[f] < 0 \Big\}.$$

Assume that A is a (not necessarily semi-bounded) self-adjoint operator in a Hilbert space $\mathcal{H}$ with the corresponding spectral measure $E_A(\cdot)$. Define the possibly non-closed quadratic form $\mathfrak{s}_A$ by

$$\mathfrak{s}_A[f] := (Af, f)_{\mathcal{H}}, \quad \operatorname{dom}\mathfrak{s}_A := \operatorname{dom} A.$$

If, in addition, A is semi-bounded, then by [K95, Theorem VI.1.27] the form $\mathfrak{s}_A$ is closable, and we denote its closure by $\overline{\mathfrak{s}_A}$. According to the spectral theorem for self-adjoint operators and [BS87, 10.2 Theorem 3]

$$\dim \operatorname{ran} E_A(-\infty, 0) = \kappa_-(\mathfrak{s}_A) = \kappa_-(\overline{\mathfrak{s}_A}). \tag{4.5.5}$$

In particular, if $\kappa_-(\mathfrak{s}_A)$ is finite, then the self-adjoint operator A has finitely many negative eigenvalues with finite multiplicities.

Now we are ready to formulate and prove the main results of this subsection. We mention that finiteness of the negative spectrum in the case of δ-potentials on hypersurfaces was also shown in [BEKS94] by other methods.

Theorem 4.33. *Let $\alpha, \beta \colon \Sigma \to \mathbb{R}$ be such that $\alpha, 1/\beta \in L^\infty(\Sigma)$ and let the self-adjoint operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ be as above. Then the following statements hold.*

(i) $\sigma_{\mathrm{ess}}(-\Delta_{\delta,\alpha}) = \sigma_{\mathrm{ess}}(-\Delta_{\delta',\beta}) = [0, \infty)$.

(ii) *The self-adjoint operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ have finitely many negative eigenvalues with finite multiplicities.*

Proof. (i) According to Theorem 4.22 (i) the resolvent difference of the self-adjoint operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\rm free}$ is compact; thus

$$\sigma_{\rm ess}(-\Delta_{\delta,\alpha}) = \sigma_{\rm ess}(-\Delta_{\rm free}) = [0,\infty).$$

Analogously, according to Theorem 4.26 (i) the resolvent difference of the self-adjoint operators $-\Delta_{\delta',\beta}$ and $-\Delta_{\rm free}$ is also compact. Hence

$$\sigma_{\rm ess}(-\Delta_{\delta',\beta}) = \sigma_{\rm ess}(-\Delta_{\rm free}) = [0,\infty).$$

(ii) Let us introduce the (in general non-closed) quadratic forms

$$\begin{aligned}
\mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] &:= \big(-\Delta_{\delta,\alpha} f, f\big), \qquad \mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}}) := \mathrm{dom}(-\Delta_{\delta,\alpha}),\\
\mathfrak{s}_{-\Delta_{\delta',\beta}}[f] &:= \big(-\Delta_{\delta',\beta} f, f\big), \quad \mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}}) := \mathrm{dom}(-\Delta_{\delta',\beta}).
\end{aligned}$$

Applying the first Green's identity (4.1.7) to these expressions and taking the definitions (4.2.6), (4.3.5) of the domains of the operators $-\Delta_{\delta,\alpha}$, $-\Delta_{\delta',\beta}$ into account we obtain

$$\begin{aligned}
\mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] &= \big(-\Delta f_{\rm i}, f_{\rm i}\big)_{\rm i} + \big(-\Delta f_{\rm e}, f_{\rm e}\big)_{\rm e}\\
&= \big(\nabla f_{\rm i}, \nabla f_{\rm i}\big)_{\rm i} - \big(\partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma, f_{\rm i}|_\Sigma\big)_\Sigma + \big(\nabla f_{\rm e}, \nabla f_{\rm e}\big)_{\rm e} - \big(\partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma, f_{\rm e}|_\Sigma\big)_\Sigma\\
&= \big(\nabla f, \nabla f\big) - \big(\alpha f|_\Sigma, f|_\Sigma\big)_\Sigma
\end{aligned}$$

and

$$\begin{aligned}
\mathfrak{s}_{-\Delta_{\delta',\beta}}[f] &= \big(-\Delta f_{\rm i}, f_{\rm i}\big)_{\rm i} + \big(-\Delta f_{\rm e}, f_{\rm e}\big)_{\rm e}\\
&= \big(\nabla f_{\rm i}, \nabla f_{\rm i}\big)_{\rm i} - \big(\partial_{\nu_{\rm i}} f_{\rm i}|_\Sigma, f_{\rm i}|_\Sigma\big)_\Sigma + \big(\nabla f_{\rm e}, \nabla f_{\rm e}\big)_{\rm e} - \big(\partial_{\nu_{\rm e}} f_{\rm e}|_\Sigma, f_{\rm e}|_\Sigma\big)_\Sigma\\
&= (\nabla f, \nabla f) + \big(\beta^{-1}(f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma), f_{\rm i}|_\Sigma\big)_\Sigma - \big(\beta^{-1}(f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma), f_{\rm e}|_\Sigma\big)_\Sigma\\
&= \big(\nabla f, \nabla f\big) - \big(\beta^{-1}(f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma), f_{\rm e}|_\Sigma - f_{\rm i}|_\Sigma\big)_\Sigma.
\end{aligned}$$

For a bounded function $\sigma\colon \Sigma \to \mathbb{R}$ define the quadratic form $\mathfrak{q}_\sigma$

$$\mathfrak{q}_\sigma[f] := \big(\nabla f, \nabla f\big) - \big(\sigma f_{\rm i}|_\Sigma, f_{\rm i}|_\Sigma\big)_\Sigma - \big(\sigma f_{\rm e}|_\Sigma, f_{\rm e}|_\Sigma\big)_\Sigma, \quad \mathrm{dom}\,\mathfrak{q}_\sigma := H^1(\mathbb{R}^n\setminus\Sigma).$$

It follows from [B62, Theorem 6.9] (cf. the proof of Proposition 4.31 above) that the form $\mathfrak{q}_\sigma$ is closed and semi-bounded, and the self-adjoint operator corresponding to $\mathfrak{q}_\sigma$ has finitely many negative eigenvalues with finite multiplicities. Thus, by (4.5.5), we have $\kappa_-(\mathfrak{q}_\sigma) < \infty$. It can easily be checked that

$$\mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}}) \subset \mathrm{dom}(\mathfrak{q}_{|\alpha|/2}) \quad \text{and} \quad \forall\, f \in \mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}})\colon \mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] \ge \mathfrak{q}_{|\alpha|/2}[f].$$

Using the inequality $|a-b|^2 \leq 2(|a|^2+|b|^2)$ for complex numbers a, b we obtain

$$\mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}}) \subset \mathrm{dom}(\mathfrak{q}_{2/|\beta|}) \quad \text{and} \quad \forall\, f \in \mathrm{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}})\colon \mathfrak{s}_{-\Delta_{\delta',\beta}}[f] \geq \mathfrak{q}_{2/|\beta|}[f].$$

These observations yield that

$$\kappa_-(\mathfrak{s}_{-\Delta_{\delta,\alpha}}) \leq \kappa_-(\mathfrak{q}_{|\alpha|/2}) < \infty \quad \text{and} \quad \kappa_-(\mathfrak{s}_{-\Delta_{\delta',\beta}}) \leq \kappa_-(\mathfrak{q}_{2/|\beta|}) < \infty.$$

From this and (4.5.5) it follows that the negative spectra of $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ are finite. $\square$

4.6 Comments

Schrödinger operators with point δ-interactions in the simplest one-dimensional case appeared already more than eighty years ago in the paper [KP31] by Kronig and Penney, where they were used in the quantum mechanical model of a charged free particle in a one-dimensional lattice. It took thirty years, until a model of a point δ-interaction in the three-dimensional case based on the operator extension theory was proposed by Berezin and Faddeev in [BF61]. An approach to point interactions in arbitrary space dimensions based on Pontryagin spaces was developed by Shondin [Sho88]. For more details on point interactions see the monographs [AGHH05, AK00] and the references therein.

Schrödinger operators with δ and δ'-potentials on hypersurfaces were investigated systematically first only in the late 80s under additional symmetry assumptions in [AGS87, Sh88] by Antoine, Gesztesy and Shabani. In these papers the main tool of analysis is the reduction to Sturm-Liouville operators via separation of variables. A rigorous approach to the definition and the spectral analysis of Schrödinger operators with δ-interactions on general hypersurfaces is provided in [BEKS94] by Brasche, Exner, Kuperin and Šeba. In particular, Krein's formula and a variant of the Birman-Schwinger principle in Theorem 4.6 are already contained in [BEKS94, Corollary 2.1 and Corollary 2.3], which are derived from the corresponding sesquilinear form, cf. Proposition 4.30.

The development of an approach to δ'-interactions on general hypersurfaces has been posed as an open problem in [E08, Open problem 7.2]. The treatment of these potentials is more involved because they are more singular. In the thesis a solution of this open problem is presented.

Schatten-von Neumann estimates for the resolvent power differences of the free operator $A_{\rm free}$ and the decoupled operators $A_{\rm D,i,e}$ and $A_{\rm N,i,e}$ were investigated by Deift and Simon [DS75, Lemma 3], Jensen and Kato [JK78], Bardos, Guillot, and Ralston [BGR82], Grubb [G84a] and more recently by Carron in [Ca02, Théorème 1.1] and by Alpay and Behrndt in [AB09, Theorem 4.4 (iii)]. It seems that analogous estimates for δ and δ'-couplings, given in Theorems 4.22, 4.25 and 4.26, were not obtained before. The trace formulae in Subsection 4.4.2 extend the corresponding trace formula in [Ca02, Théorème 2.2] to the case of δ and δ'-couplings.

The proof of finiteness of the negative spectra for the operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ in Theorem 4.33 is reduced to a result by Birman [B62, Theorem 6.9], which states finiteness of negative spectra of Robin Laplacians on exterior domains. In the case of δ-interactions finiteness of negative spectra can also be deduced from the spectral estimates in [BEKS94, Theorem 4.2 (iii)]. The operator $-\Delta_{\delta',\beta}$ with β having unbounded inverse can be treated as in Marletta and Rosenblum [MR09], and in this case the number of negative eigenvalues can be infinite.

Finally, we mention some of the recent significant papers in the area of interactions supported on hypersurfaces: Brown, Eastham, and Wood [BEW09], Exner [E03, E05], Exner and Fraas [EF09], Exner and Ichinose [EI01], Exner and Kondej [EK02, EK03], Exner and Yoshitomi [EY02], Kondej and Veselic [KV07] for studies of eigenvalues; Birman, Shterenberg, and Suslina [BSS00], Exner and Fraas [EF07], Exner and Yoshitomi [EY01], Suslina and Shterenberg [SuSh01] for results on the absolutely continuous spectrum; Exner and his co-authors [EK05, EN03, EY02a, EY04] for related problems on Schrödinger operators with δ-interactions. The contents of these papers are partially reviewed in [E08], see also the references in this review paper.

Chapter 5

Robin Laplacians on a half-space

In this chapter we define self-adjoint Laplace operators on a half-space subject to Robin and more general non-local self-adjoint boundary conditions. We provide an analogue of the Birman-Schwinger principle for the characterization of the point spectra and Krein's formula for the resolvent differences.

Furthermore, we give a sufficient condition for H^2-regularity of the operator domains. As the underlying problem of this chapter we study compactness of the resolvent differences and Schatten-von Neumann properties of the resolvent power differences of self-adjoint Robin Laplacians. The non-compactness of the boundary leads to serious changes in the proofs in comparison with the previous chapters. The Schatten-von Neumann estimates in this chapter complement the works [B62, GorK82, DM91]. The material of this chapter is partially contained in the work of the author [LR12].

5.1 Preliminaries

Let $\mathbb{R}^n_+$, $n \geq 2$, be the half-space $\{(x', x_n)^\top : x' \in \mathbb{R}^{n-1}, x_n \in \mathbb{R}_+\}$ with the boundary $\partial\mathbb{R}^n_+$. We denote by $(\cdot,\cdot)$ and $(\cdot,\cdot)_{\partial\mathbb{R}^n_+}$ the inner products in the Hilbert spaces $L^2(\mathbb{R}^n_+)$ and $L^2(\partial\mathbb{R}^n_+)$, respectively. Throughout this chapter we deal with the Laplace differential expression on $\mathbb{R}^n_+$. For a function $f \in C^\infty(\overline{\mathbb{R}^n_+})$ we introduce the following trace

$$\partial_\nu f|_{\partial\mathbb{R}^n_+} := -\partial_{x_n} f|_{\partial\mathbb{R}^n_+}.$$

For $s > 3/2$ the trace mapping

$$H^s(\mathbb{R}^n_+) \ni f \mapsto \{f|_{\partial\mathbb{R}^n_+}, \partial_\nu f|_{\partial\mathbb{R}^n_+}\} \in H^{s-1/2}(\partial\mathbb{R}^n_+) \times H^{s-3/2}(\partial\mathbb{R}^n_+) \tag{5.1.1}$$

is the extension by continuity of the trace mapping defined on C^∞-functions and the mapping in (5.1.1) is surjective onto $H^{s-1/2}(\partial\mathbb{R}^n_+) \times H^{s-3/2}(\partial\mathbb{R}^n_+)$. Besides the Sobolev spaces $H^s(\mathbb{R}^n_+)$ defined in Section 2.3 we also actively employ the spaces

$$H^s_\Delta(\mathbb{R}^n_+) := \{f \in H^s(\mathbb{R}^n_+) \colon \Delta f \in L^2(\mathbb{R}^n_+)\}, \quad s \geq 0. \tag{5.1.2}$$

Observe that for $s \geq 2$ the spaces $H^s_\Delta(\mathbb{R}^n_+)$ and $H^s(\mathbb{R}^n_+)$ coincide. We also note that for $s \in (0,2)$ the space $H^s_\Delta(\mathbb{R}^n_+)$ can be viewed as an interpolation space between $H^2(\mathbb{R}^n_+)$ and $H^0_\Delta(\mathbb{R}^n_+)$. By [F67] the trace mapping admits an extension by continuity to the mapping

$$H^s_\Delta(\mathbb{R}^n_+) \ni f \mapsto \{f|_{\partial\mathbb{R}^n_+}, \partial_\nu f|_{\partial\mathbb{R}^n_+}\} \in H^{s-1/2}(\partial\mathbb{R}^n_+) \times H^{s-3/2}(\partial\mathbb{R}^n_+), \tag{5.1.3}$$

with $s \in [0,2)$, where the mappings

$$\begin{aligned} H^s_\Delta(\mathbb{R}^n_+) \ni f \mapsto f|_{\partial\mathbb{R}^n_+} \in H^{s-1/2}(\partial\mathbb{R}^n_+), \quad s \in [0,2), \\ H^s_\Delta(\mathbb{R}^n_+) \ni f \mapsto \partial_\nu f|_{\partial\mathbb{R}^n_+} \in H^{s-3/2}(\partial\mathbb{R}^n_+), \quad s \in [0,2), \end{aligned} \tag{5.1.4}$$

are surjective onto $H^{s-1/2}(\partial\mathbb{R}^n_+)$ and onto $H^{s-3/2}(\partial\mathbb{R}^n_+)$, respectively. We also recall that for $f, g \in H^{3/2}_\Delta(\mathbb{R}^n_+)$ the second Green's identity

$$\big(-\Delta f, g\big) - \big(f, -\Delta g\big) = \big(f|_{\partial\mathbb{R}^n_+}, \partial_\nu g|_{\partial\mathbb{R}^n_+}\big)_{\partial\mathbb{R}^n_+} - \big(g|_{\partial\mathbb{R}^n_+}, \partial_\nu f|_{\partial\mathbb{R}^n_+}\big)_{\partial\mathbb{R}^n_+} \tag{5.1.5}$$

holds.

The minimal symmetric operator

$$Af := -\Delta f, \quad \operatorname{dom} A := H^2_0(\mathbb{R}^n_+),$$

is closed and densely defined in $L^2(\mathbb{R}^n_+)$ with the adjoint of the form

$$A^* f = -\Delta f, \quad \operatorname{dom} A^* = H^0_\Delta(\mathbb{R}^n_+).$$

Self-adjoint extensions of A subject to Dirichlet and Neumann boundary conditions

$$\begin{aligned} A_{\mathrm{D}} f &:= -\Delta f, \quad \operatorname{dom} A_{\mathrm{D}} := \{f \in H^2(\mathbb{R}^n_+) \colon f|_{\partial\mathbb{R}^n_+} = 0\}, \\ A_{\mathrm{N}} f &:= -\Delta f, \quad \operatorname{dom} A_{\mathrm{N}} := \{f \in H^2(\mathbb{R}^n_+) \colon \partial_\nu f|_{\partial\mathbb{R}^n_+} = 0\} \end{aligned} \tag{5.1.6}$$

will be actively used further. For the proof of their self-adjointness we refer to [G09, Chapter 9].

5.2 Half-space Laplacians with general self-adjoint boundary conditions

In this section we make use of quasi boundary triples for a proper definition and study of self-adjoint realizations $A_{[B]}$ of $-\Delta$ subject to a non-local boundary condition

$$Bf|_{\partial\mathbb{R}^n_+} = \partial_\nu f|_{\partial\mathbb{R}^n_+}$$

with a bounded self-adjoint operator B in $L^2(\partial\mathbb{R}^n_+)$.

5.2.1 A quasi boundary triple and its Weyl function

For a definition of a quasi boundary triple for A^* we specify the operator T as below

$$Tf := -\Delta f, \quad \operatorname{dom} T := H^{3/2}_\Delta(\mathbb{R}^n_+), \tag{5.2.1}$$

where the space $H^{3/2}_\Delta(\mathbb{R}^n_+)$ is defined in (5.1.2). We require also the boundary mappings

$$\begin{aligned} &\Gamma_0\colon \operatorname{dom} T \to L^2(\partial\mathbb{R}^n_+), \quad \Gamma_0 f := \partial_\nu f|_{\partial\mathbb{R}^n_+},\\ &\Gamma_1\colon \operatorname{dom} T \to L^2(\partial\mathbb{R}^n_+), \quad \Gamma_1 f := f|_{\partial\mathbb{R}^n_+}. \end{aligned} \tag{5.2.2}$$

In the first proposition of this section we prove that $\{L^2(\partial\mathbb{R}^n_+), \Gamma_0, \Gamma_1\}$ is a quasi boundary for A^* and we show some basic properties of this quasi boundary triple.

Proposition 5.1. *Let the self-adjoint operators A_N and A_D be as in (5.1.6). Let the operator T be as in (5.2.1) and the mappings Γ_0, Γ_1 be as in (5.2.2). Then the triple $\Pi = \{L^2(\partial\mathbb{R}^n_+), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^*. The restrictions of T to the kernels of the boundary mappings are*

$$T \upharpoonright \ker\Gamma_0 = A_\mathrm{N} \quad \textit{and} \quad T \upharpoonright \ker\Gamma_1 = A_\mathrm{D};$$

and the ranges of these mappings are

$$\operatorname{ran}\Gamma_0 = L^2(\partial\mathbb{R}^n_+) \quad \textit{and} \quad \operatorname{ran}\Gamma_1 = H^1(\partial\mathbb{R}^n_+).$$

Proof. In order to show that the triple Π is a quasi boundary triple for A^* we use Proposition 2.9. Let us check that the triple Π satisfies the conditions (a), (b) and (c) of that proposition. Since $H^2(\mathbb{R}^n_+) \subset \operatorname{dom} T$, by (5.1.1) we have

$$H^{1/2}(\partial\mathbb{R}^n_+) \times H^{3/2}(\partial\mathbb{R}^n_+) \subset \operatorname{ran}\begin{pmatrix}\Gamma_0\\ \Gamma_1\end{pmatrix}.$$

The set $H^{1/2}(\partial\mathbb{R}^n_+) \times H^{3/2}(\partial\mathbb{R}^n_+)$ is clearly dense in $L^2(\partial\mathbb{R}^n_+) \times L^2(\partial\mathbb{R}^n_+)$. Note that also the set $\ker\Gamma_0 \cap \ker\Gamma_1 \supset C_0^\infty(\mathbb{R}^n_+)$ is dense in $L^2(\mathbb{R}^n_+)$. Thus the condition (a) is verified. The abstract Green's identity

$$\big(Tf, g\big) - \big(f, Tg\big) = \big(\Gamma_1 f, \Gamma_0 g\big)_{\partial\mathbb{R}^n_+} - \big(\Gamma_0 f, \Gamma_1 g\big)_{\partial\mathbb{R}^n_+}$$

for all $f, g \in \operatorname{dom} T$ is equivalent to (5.1.5). The condition (b) is also checked. The operator $T \upharpoonright \ker\Gamma_0$ contains the self-adjoint Laplacian A_{N} subject to Neumann boundary condition on $\partial\mathbb{R}^n_+$. Thus the condition (c) holds for the triple Π. Therefore, by Proposition 2.9 the triple Π is a quasi boundary triple for the adjoint of the closed symmetric operator $T \upharpoonright \big(\ker\Gamma_0 \cap \ker\Gamma_1\big)$.

It remains to show that $T \upharpoonright \big(\ker\Gamma_0 \cap \ker\Gamma_1\big) = A$. The operator $T \upharpoonright \ker\Gamma_0$ contains the self-adjoint operator A_{N} and the operator $T \upharpoonright \ker\Gamma_1$ contains the self-adjoint operator A_{D}. By the abstract Green's identity the operators $T \upharpoonright \ker\Gamma_0$ and $T \upharpoonright \ker\Gamma_1$ are both symmetric, thus $T \upharpoonright \ker\Gamma_0 = A_{\mathrm{N}}$ and $T \upharpoonright \ker\Gamma_1 = A_{\mathrm{D}}$. As a consequence

$$T \upharpoonright \big(\ker\Gamma_0 \cap \ker\Gamma_1\big) = \big(T \upharpoonright \ker\Gamma_0\big) \cap \big(T \upharpoonright \ker\Gamma_1\big) = A_{\mathrm{N}} \cap A_{\mathrm{D}} = A.$$

Hence the triple Π is a quasi boundary triple for A^*.

The properties of the boundary mappings

$$\operatorname{ran}\Gamma_0 = L^2(\partial\mathbb{R}^n_+) \quad \text{and} \quad \operatorname{ran}\Gamma_1 = H^1(\partial\mathbb{R}^n_+)$$

follow from (5.1.4) ☐

In the next proposition we clarify the basic properties of the γ-field and the Weyl function associated with the quasi boundary triple Π from Proposition 5.1. In the terminology of [G09], these operators turn out to be the Poisson operator and the Neumann-to-Dirichlet map, respectively.

Proposition 5.2. *Let the self-adjoint operators A_{D} and A_{N} be as in (5.1.6). Let Π be the quasi boundary triple from Proposition 5.1. Let γ and M be, respectively, the γ-field and the Weyl function associated with the quasi boundary triple Π. Then the following statements hold.*

(i) *The γ-field γ is defined for all $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ and*

$$\gamma(\lambda)\colon L^2(\partial\mathbb{R}^n_+) \to L^2(\mathbb{R}^n_+), \quad \gamma(\lambda)f = f_\lambda(\varphi),$$

where $f_\lambda(\varphi)$ is the unique solution in the space $H^{3/2}_\Delta(\mathbb{R}^n_+)$ of the problem

$$\begin{aligned} (-\Delta - \lambda)f &= 0, \quad \textit{in } \mathbb{R}^n_+, \\ \partial_\nu f|_{\partial\mathbb{R}^n_+} &= \varphi, \quad \textit{on } \partial\mathbb{R}^n_+. \end{aligned}$$

(ii) *The Weyl function M is defined for all $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ and*

$$M(\lambda)\colon L^2(\partial\mathbb{R}^n_+) \to L^2(\partial\mathbb{R}^n_+), \quad M(\lambda)\varphi = f_\lambda(\varphi)|_{\partial\mathbb{R}^n_+},$$

where $f_\lambda(\varphi) = \gamma(\lambda)\varphi$. The operator $M(\lambda)$ maps $L^2(\partial\mathbb{R}^n_+)$ onto $H^1(\partial\mathbb{R}^n_+)$. For $\lambda < 0$ it holds that $\|M(\lambda)\| \le \frac{1}{\sqrt{-\lambda}}$, and, in particular, the limit property

$$\lim_{\lambda\to-\infty} \big\|M(\lambda)\big\| = 0$$

holds.

Proof. As a preliminary step, note that $\sigma(A_\mathrm{D}) = \sigma(A_\mathrm{N}) = \mathbb{R}_+$ and thus $\mathbb{C} \setminus \mathbb{R}_+ = \rho(A_\mathrm{D}) \cap \rho(A_\mathrm{N})$.

(i) The mapping properties of the γ-field γ follow from (5.2.1), (5.2.2) and Definition 2.10.

(ii) The mapping properties of the Weyl function follow from (5.2.2), Definition 2.10, Proposition 2.11 (iii), and Proposition 5.1.

For $\lambda < 0$ the Weyl function M can be represented as

$$M(\lambda) = (-\Delta_{\mathbb{R}^{n-1}} - \lambda)^{-1/2},$$

where $-\Delta_{\mathbb{R}^{n-1}}$ is the standard self-adjoint Laplace operator in $L^2(\mathbb{R}^{n-1})$ with the usual domain $H^2(\mathbb{R}^{n-1})$, see, e.g., [G09, Chapter 9]. As a consequence of this representation we obtain

$$\big\|M(\lambda)\big\| \le \frac{1}{\sqrt{-\lambda}},$$

and the limit property follows automatically. $\square$

5.2.2 Self-adjointness and Krein's formulae

In the next theorem we provide a factorization (Krein's formula) for the resolvent difference of the self-adjoint operators A_N and A_D.

Theorem 5.3. *Let A_N and A_D be the self-adjoint operators as in (5.1.6). Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Then the formula*

$$(A_\mathrm{N} - \lambda)^{-1} - (A_\mathrm{D} - \lambda)^{-1} = \gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^*$$

holds for all $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$.

Proof. Krein's formula follows from Theorem 2.13 (ii) with $A_0 = A_\mathrm{N}$ and $A_1 = A_\mathrm{D}$. $\square$

Further, we define Laplace operators on the half-space with non-local boundary conditions.

Definition 5.4. For a bounded self-adjoint operator B in $L^2(\partial\mathbb{R}^n_+)$ we define the restriction $A_{[B]}$ of T as below

$$A_{[B]} := T \upharpoonright \ker(B\Gamma_1 - \Gamma_0), \tag{5.2.3}$$

which is equivalent to

$$A_{[B]} = -\Delta f, \quad \operatorname{dom} A_{[B]} = \left\{ f \in H^{3/2}_\Delta(\mathbb{R}^n_+) \colon Bf|_{\partial\mathbb{R}^n_+} = \partial_\nu f|_{\partial\mathbb{R}^n_+} \right\}.$$

$$\begin{array}{ccccccccc}
 & & A_\mathrm{N} & & & & & & \\
 & \rotatebox{45}{$\subset$} & & \rotatebox{-45}{$\subset$} & & & & & \\
A & \subset & A_{[B]} & \subset & T & \subset & \overline{T} & = & A^*. \\
 & \rotatebox{-45}{$\subset$} & & \rotatebox{45}{$\subset$} & & & & & \\
 & & A_\mathrm{D} & & & & & &
\end{array}$$

Figure 5.1: This figure shows how the operator $A_{[B]}$ is related to the other operators introduced in this chapter. The operators A_N, A_D and $A_{[B]}$ are self-adjoint in $L^2(\mathbb{R}^n_+)$, cf. Theorem 5.5.

In the next theorem we show that the operator $A_{[B]}$ is self-adjoint. Moreover, we establish a characterization of the point spectrum of $A_{[B]}$ in terms of the point spectrum of the operator-valued function $I - BM(\cdot)$ and we provide a factorization for the resolvent difference of $A_{[B]}$ and A_{N}.

Theorem 5.5. *Let A_{N} be the self-adjoint operator as in (5.1.6). Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Let B be a bounded self-adjoint operator in $L^2(\partial\mathbb{R}^n_+)$. Let $A_{[B]}$ be the operator corresponding to B via (5.2.3). Then the following statements hold.*

(i) *The operator $A_{[B]}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R}^n_+)$ and*

$$A_{[B]} \geq -\|B\|^2.$$

(ii) *For all $\lambda \in \mathbb{R}_-$*

$$\lambda \in \sigma_{\mathrm{p}}(A_{[B]}) \quad \Longleftrightarrow \quad 0 \in \sigma_{\mathrm{p}}\big(I - BM(\lambda)\big),$$

and the multiplicities of these eigenvalues coincide.

(iii) *The formula*

$$(A_{[B]} - \lambda)^{-1} - (A_{\mathrm{N}} - \lambda)^{-1} = \gamma(\lambda)\big(I - BM(\lambda)\big)^{-1} B\gamma(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{[B]}) \cap \rho(A_{\mathrm{N}})$.

Proof. (i) By Proposition 5.1 the range of the boundary mapping Γ_0 coincides with the auxiliary Hilbert space $L^2(\partial\mathbb{R}^n_+)$. By assumptions the operator B is bounded and self-adjoint in $L^2(\partial\mathbb{R}^n_+)$. Hence, by Proposition 5.2 (ii) for all $\lambda < -\|B\|^2$ the condition

$$\|M(\lambda)\| \cdot \|B\| < 1,$$

holds, and Theorem 2.21 implies the statement.

(ii) The equivalence between the point spectra is a consequence of Proposition 2.14.

(iii) Krein's formula follows from Corollary 2.16 in view of the self-adjointness of $A_{[B]}$. $\square$

In the next theorem we obtain a factorization (Krein's formula) for the resolvent difference of $A_{[B_1]}$ and $A_{[B_2]}$.

Theorem 5.6. *Let A_{N} be the self-adjoint operator from (5.1.6), and let γ and M be the γ-field and the Weyl function from Proposition 5.2. Let B_1 and B_2 be bounded self-adjoint operators in $L^2(\partial\mathbb{R}^n_+)$, and let $A_{[B_1]}$ and $A_{[B_2]}$ be the self-adjoint operators corresponding via (5.2.3) to B_1 and B_2, respectively. Then the formula*

$$(A_{[B_2]} - \lambda)^{-1} - (A_{[B_1]} - \lambda)^{-1} = \gamma(\lambda)\big(I - B_2 M(\lambda)\big)^{-1}(B_2 - B_1)\big(I - M(\lambda)B_1\big)^{-1}\gamma(\overline{\lambda})^*$$

holds for all $\lambda \in \rho(A_{[B_2]}) \cap \rho(A_{[B_1]}) \cap \rho(A_{\mathrm{N}})$. In this formula the middle terms satisfy

$$(I - B_2 M(\lambda))^{-1}, (I - M(\lambda)B_1)^{-1} \in \mathcal{B}(L^2(\partial\mathbb{R}^n_+))$$

for all $\lambda \le -\max\{\|B_1\|^2, \|B_2\|^2\}$.

Proof. Krein's formula follows from Theorem 2.17, and self-adjointness of $A_{[B_1]}$ and $A_{[B_2]}$. According to Proposition 4.2 (ii) we immediately get for all $\lambda < -\max\{\|B_1\|^2, \|B_2\|^2\}$ the inequalities $\|B_i M(\lambda)\| < 1$ with $i = 1, 2$, which imply the properties of the middle terms. $\square$

Furthermore, we formulate an analogue of Theorem 3.7 for the half-space case with analogous proof which is omitted.

Theorem 5.7. *Let B be a bounded self-adjoint operator in $L^2(\partial\mathbb{R}^n_+)$, and let $A_{[B]}$ be the operator corresponding to B via (5.2.3). Assume that*

$$f \in H^1(\partial\mathbb{R}^n_+) \quad \Longrightarrow \quad Bf \in H^{1/2}(\partial\mathbb{R}^n_+).$$

Then the inclusion $\operatorname{dom} A_{[B]} \subset H^2(\mathbb{R}^n_+)$ *holds.*

If B is an operator of multiplication with a real-valued bounded function β, then we agree to write $A_{[\beta]}$ instead of $A_{[B]}$.

Corollary 5.8. *Assume that $\beta \in W^{1,\infty}(\partial\mathbb{R}^n_+)$. Then the inclusion* $\operatorname{dom} A_{[\beta]} \subset H^2(\mathbb{R}^n_+)$ *holds.*

5.3 Operator ideal properties of resolvent power differences and trace formulae

Throughout this section we focus only on self-adjoint extensions with local Robin boundary conditions, namely

$$(5.3.1)\quad A_{[\beta]} f := -\Delta f, \quad \operatorname{dom} A_{[\beta]} := \big\{ f \in H^{3/2}_{\Delta}(\mathbb{R}^n_+) \colon \beta f|_{\partial\mathbb{R}^n_+} = \partial_\nu f|_{\partial\mathbb{R}^n_+} \big\},$$

where β is a real-valued L^∞-function. We obtain sufficient conditions on $\beta_2-\beta_1$ ensuring compactness or certain Schatten-von Neumann properties of the resolvent differences or the resolvent power differences of the self-adjoint operators $A_{[\beta_1]}$ and $A_{[\beta_2]}$. For the trace class resolvent power differences we provide the corresponding trace formulae.

5.3.1 Compactness of resolvent differences

In this subsection we give a sufficient condition on $\beta_2-\beta_1$ for compactness of the resolvent difference of $A_{[\beta_1]}$ and $A_{[\beta_2]}$. This condition includes the case of uniformly vanishing $\beta_2 - \beta_1$ with respect to all directions and also more general situations. In the particular case $\beta_1 \equiv 0$, i.e. $A_{[\beta_1]} = A_{\mathrm{N}}$, we pass to the conclusions about the absolutely continuous parts of the operators using recent results of the work [MN11].

Let us recall condition (2.3.6) on a function $\alpha \in L^\infty(\partial\mathbb{R}^n_+)$, which is given first in Subsection 2.3.2, namely

$$\mu\left(\left\{x \in \partial\mathbb{R}^n_+ : |\alpha(x)| \geq \varepsilon\right\}\right) < \infty, \quad \text{for all } \varepsilon > 0, \tag{5.3.2}$$

here μ denotes the Lebesgue measure on $\partial\mathbb{R}^n_+$.

Theorem 5.9. *Let real-valued $\beta_1, \beta_2 \in L^\infty(\partial\mathbb{R}^n_+)$ be such that $\beta := \beta_2 - \beta_1$ satisfies condition (5.3.2), and let $A_{[\beta_1]}$ and $A_{[\beta_2]}$ be the self-adjoint Robin Laplacians on the half-space corresponding via (5.3.1) to β_1 and β_2, respectively. Then the following property*

$$(A_{[\beta_2]} - \lambda)^{-1} - (A_{[\beta_1]} - \lambda)^{-1} \in \mathfrak{S}_\infty(L^2(\mathbb{R}^n_+))$$

holds for all $\lambda \in \rho(A_{[\beta_2]}) \cap \rho(A_{[\beta_1]})$.

Proof. Let us fix $\lambda_0 < -\max\{\|\beta_1\|^2_\infty, \|\beta_2\|^2_\infty\}$. Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Theorem 5.6 claims, among other, that

$$\big(I - \beta_2 M(\lambda_0)\big)^{-1}, \big(I - M(\lambda_0)\beta_1\big)^{-1} \in \mathcal{B}\big(L^2(\partial\mathbb{R}^n_+)\big). \tag{5.3.3}$$

Note that the mapping Γ_0 is surjective onto $L^2(\partial\mathbb{R}^n_+)$, hence, by Proposition 2.11 (i)

$$\gamma(\lambda_0) \in \mathcal{B}\big(L^2(\partial\mathbb{R}^n_+), L^2(\mathbb{R}^n_+)\big), \tag{5.3.4}$$

and the adjoint of $\gamma(\lambda_0)$ can be represented as

$$\gamma(\lambda_0)^* = \Gamma_1(A_{\mathrm{N}} - \lambda_0)^{-1}.$$

Note that $\operatorname{ran}((A_{\mathrm{N}}-\lambda_0)^{-1}) \subset H^2(\mathbb{R}^n_+)$ and that Γ_1 is the usual trace. Thus, by (5.1.1) it holds that

$$\operatorname{ran}(\gamma(\lambda_0)^*) \subset H^{3/2}(\partial\mathbb{R}^n_+) \subset H^1(\partial\mathbb{R}^n_+). \tag{5.3.5}$$

According to Proposition 5.2 (ii), we get

$$\operatorname{ran} M(\lambda_0) = H^1(\partial\mathbb{R}^n_+). \tag{5.3.6}$$

Note that in view of (5.3.3) for an arbitrary $\psi \in L^2(\partial\mathbb{R}^n_+)$ the element

$$\varphi := \big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^*\psi$$

is well-defined. Applying the operator $I - M(\lambda_0)\beta_1$ to both hand sides in the last equation, we obtain using (5.3.5) and (5.3.6) that

$$\varphi = \gamma(\lambda_0)^*\psi + M(\lambda_0)\beta_1\varphi \in H^1(\partial\mathbb{R}^n_+).$$

Now Lemma 2.23 and the assumptions on β yield

$$\beta\big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^* \in \mathfrak{S}_\infty\big(L^2(\mathbb{R}^n_+), L^2(\partial\mathbb{R}^n_+)\big). \tag{5.3.7}$$

According to the factorization from Theorem 5.6 with $B_1 = \beta_1$ and $B_2 = \beta_2$

$$\begin{aligned}(A_{[\beta_2]} - \lambda_0)^{-1} &- (A_{[\beta_1]} - \lambda_0)^{-1}\\ &= \gamma(\lambda)\big(I - \beta_2 M(\lambda_0)\big)^{-1}\beta\big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^*,\end{aligned}$$

and using (5.3.3), (5.3.4) and (5.3.7) we get the claim for the point $\lambda = \lambda_0$. Finally, applying Lemma 2.2 with $m = 1$ and $\mathfrak{A} = \mathfrak{S}_\infty$ we get the statement for all $\lambda \in \rho(A_{[\beta_2]}) \cap \rho(A_{[\beta_1]})$. $\square$

The corollary below follows from the theorem above and [MN11, Proposition 5.11 (v) and (vii)]

Corollary 5.10. *Let the self-adjoint operator A_{N} be as in (5.1.6). Let a real-valued $\beta \in L^\infty(\partial\mathbb{R}^n)$ satisfy the condition (5.3.2), and let $A_{[\beta]}$ be the self-adjoint Robin Laplacian on the half-space corresponding to β via (5.3.1). Then the operator A_{N} and the absolutely continuous part of the operator $A_{[\beta]}$ are unitarily equivalent.*

5.3.2 Elliptic regularity and related $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$-estimates

In this subsection we obtain regularity of the functions $(A_{[\beta]} - \lambda)^{-1} f$ under certain assumptions on the smoothness of f and β. These results are then used to obtain estimates of singular values for certain compact operators appearing in the representation of resolvent power differences of the self-adjoint operators $A_{[\beta_2]}$ and $A_{[\beta_1]}$.

In the next lemma we show smoothing properties of the γ-field γ and the Weyl function M from Proposition 5.2.

Lemma 5.11. *Let the self-adjoint operator A_{N} be as in (5.1.6). Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Then the following smoothing properties*

$$\begin{aligned} \operatorname{ran}\big(\gamma(\lambda) \upharpoonright H^s(\partial\mathbb{R}^n_+)\big) &\subset H^{s+3/2}(\mathbb{R}^n_+), \\ \operatorname{ran}\big(M(\lambda) \upharpoonright H^s(\partial\mathbb{R}^n_+)\big) &\subset H^{s+1}(\partial\mathbb{R}^n_+), \end{aligned}$$

hold for all $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ and all $s \geq 0$.

Proof. Let us fix $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$. According to the decomposition

$$\operatorname{dom} T = \operatorname{dom} A_{\mathrm{N}} \dotplus \ker(T - \lambda),$$

and, in view of (5.1.1) and (5.1.4), the mapping Γ_0 is a bijection from $H^{s+3/2}(\mathbb{R}^n_+) \cap \ker(T - \lambda)$ onto $H^s(\partial\mathbb{R}^n_+)$. Hence we conclude from Definition 2.10 that the first smoothing property holds. Since $M(\lambda) = \Gamma_1\gamma(\lambda)$ and Γ_1 is the usual trace, we get the second smoothing property from (5.1.1). $\square$

Let the spaces $W^{k,\infty}(\partial\mathbb{R}^n)$, $k \in \mathbb{N}_0$, be defined as in Section 2.3. In the next lemma we prove a more involved smoothing property. This smoothing property plays an important role in the further considerations.

Lemma 5.12. *Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Let $\beta \in W^{m,\infty}(\partial\mathbb{R}^n)$ be real-valued with $m \in \mathbb{N}$. Then the smoothing property*

$$\operatorname{ran}\Big(\big(I - M(\lambda)\beta\big)^{-1}\gamma(\lambda)^* \upharpoonright H^s(\mathbb{R}^n_+)\Big) \subset H^{s+3/2}(\partial\mathbb{R}^n_+)$$

holds for all $\lambda < -\|\beta\|_\infty^2$ and all $s \in \big[0, m - \frac{1}{2}\big]$.

Proof. Let us fix $\lambda_0 < -\|\beta\|^2_\infty$, and let us take an arbitrary $\psi \in H^s(\mathbb{R}^n_+)$. Recall that A_{N} is the realization of the Laplace differential expression on the half-space subject to the Neumann boundary condition, and thus $\lambda_0 \in \rho(A_{\mathrm{N}})$. Elliptic regularity of the Neumann Laplacian on the half-space, see, e.g. [W87, Lemma 13.1], yields

$$(A_{\mathrm{N}} - \lambda_0)^{-1}\psi \in H^{s+2}(\mathbb{R}^n_+). \tag{5.3.8}$$

By Proposition 2.11 (i) with $A_0 = A_{\mathrm{N}}$ we can express $\gamma(\lambda_0)^*$ as

$$\gamma(\lambda_0)^* = \Gamma_1(A_{\mathrm{N}} - \lambda_0)^{-1}.$$

In view of the last expression, the property of the trace (5.1.1) and the smoothing property (5.3.8) we get

$$\gamma(\lambda_0)^*\psi \in H^{s+3/2}(\partial\mathbb{R}^n_+). \tag{5.3.9}$$

According to our choice of λ_0 we obtain by Theorem 5.6 that the operator $(I - M(\lambda_0)\beta)^{-1} \in \mathcal{B}(L^2(\partial\mathbb{R}^n_+))$, and thus the element

$$\varphi := \big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*\psi$$

is well-defined. Applying the operator $I - M(\lambda_0)\beta$ to both hand sides of the last equation we get

$$\varphi = \gamma(\lambda_0)^*\psi + M(\lambda_0)\beta\varphi. \tag{5.3.10}$$

Suppose that $\varphi \in H^l(\partial\mathbb{R}^n_+)$ with some $l \in [0, m] \cap \mathbb{N}_0$. According to the assumptions on β we conclude that $\beta\varphi \in H^l(\partial\mathbb{R}^n_+)$. Furthermore, by Lemma 5.11

$$M(\lambda)\beta\varphi \in H^{l+1}(\partial\mathbb{R}^n_+). \tag{5.3.11}$$

Finally, the equation (5.3.10) and the smoothing properties (5.3.9) and (5.3.11) give the following rule:

$$\varphi \in H^l(\partial\mathbb{R}^n_+) \quad \Longrightarrow \quad \varphi \in H^{\min\{l+1, s+3/2\}}(\partial\mathbb{R}^n_+),$$

which is true for all $l = 0, 1, 2, \ldots, m$. Note that $s + 3/2 \leq m + 1$. We start from $l = 0$, and, following the rule above, we get in the end that $\varphi \in H^{s+3/2}(\partial\mathbb{R}^n_+)$, which is equivalent to our claim. $\square$

In the next lemma we prove smoothing property for the Robin Laplacian $A_{[\beta]}$ under some assumptions on the coefficient β in the boundary condition.

Lemma 5.13. *Let $\beta \in W^{m,\infty}(\partial\mathbb{R}^n_+)$ be real-valued with $m \in \mathbb{N}$, and let $A_{[\beta]}$ be the self-adjoint Robin Laplacian corresponding to β via (5.3.1). Then the smoothing property*

$$\operatorname{ran}\big((A_{[\beta]} - \lambda)^{-1} \upharpoonright H^s(\mathbb{R}^n_+)\big) \subset H^{s+2}(\partial\mathbb{R}^n_+)$$

holds for all $\lambda < -\|\beta\|^2_\infty$ and all $s \in \big[0, m - \frac{1}{2}\big]$.

Proof. Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Let us fix $\lambda_0 < -\|\beta\|^2_\infty$, and let us take an arbitrary $\psi \in H^s(\mathbb{R}^n_+)$. By Theorem 5.5 (i) the operator $A_{[\beta]}$ is self-adjoint in $L^2(\mathbb{R}^n_+)$ and, in addition, it holds that $\lambda_0 \in \rho(A_{[\beta]}) \cap \rho(A_{\mathrm{N}})$. By Lemma 4.15, with the assumption on β taken into account, we observe that

$$\big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*\psi \in H^{s+3/2}(\partial\mathbb{R}^n_+).$$

Since $s + 1/2 \leq m$, the last observation, the assumption on β and (2.3.1) yield

$$\beta\big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*\psi \in H^{s+1/2}(\partial\mathbb{R}^n_+).$$

Applying the γ-field, we get by Lemma 5.12

$$\gamma(\lambda_0)\beta\big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*\psi \in H^{s+2}(\mathbb{R}^n_+).$$

Note that $(A_{\mathrm{N}} - \lambda_0)^{-1}\psi \in H^{s+2}(\mathbb{R}^n_+)$ as well. By Krein's formula, provided in Theorem 5.6, with $B_1 = \beta$ and $B_2 = 0$ we get

$$\begin{aligned}(A_{[\beta]} - \lambda_0)^{-1}\psi &= \\ &= \underbrace{(A_{\mathrm{N}} - \lambda_0)^{-1}\psi}_{\in H^{s+2}(\mathbb{R}^n_+)} + \underbrace{\gamma(\lambda_0)\beta\big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*\psi}_{\in H^{s+2}(\mathbb{R}^n_+)} \in H^{s+2}(\mathbb{R}^n_+),\end{aligned}$$

which is equivalent to the claim because $\psi \in H^s(\mathbb{R}^n_+)$ is arbitrary. $\square$

The proposition below is the key result of this subsection and it plays a prominent role in the proof of the main results in this chapter.

Proposition 5.14. *Let the self-adjoint operator A_{N} be as in (5.1.6). Let γ and M be the γ-field and the Weyl function from Proposition 5.2. Let $\beta \in W^{2m-1,\infty}(\partial\mathbb{R}^n_+)$ with $m \in \mathbb{N}$ and $\alpha \in L^\infty(\partial\mathbb{R}^n_+)$ be real-valued, and let $A_{[\beta]}$ be the self-adjoint Robin Laplacian corresponding to β via (5.3.1). Then for $k = 0, 1, 2, \ldots, m-1$ and $\lambda < -\|\beta\|^2_\infty$ the following holds.*

(i) *If α is compactly supported, or at least $\alpha \in L^{\frac{n-1}{2k+3/2}}(\partial\mathbb{R}^n_+)$ with $\frac{n-1}{2k+3/2} > 2$, then*

$$\alpha\big(I - M(\lambda)\beta\big)^{-1}\gamma(\lambda)^*(A_{[\beta]} - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\mathbb{R}^n_+), L^2(\partial\mathbb{R}^n_+)\big),$$
$$(A_{[\beta]} - \lambda)^{-k}\gamma(\lambda)\big(I - \beta M(\lambda)\big)^{-1}\alpha \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}\big(L^2(\partial\mathbb{R}^n_+), L^2(\mathbb{R}^n_+)\big).$$

(ii) *If $\alpha \in L^p(\partial\mathbb{R}^n_+)$ with $p \geq 2$ such that $p > \frac{n-1}{2k+3/2}$, then*

$$\alpha\big(I - M(\lambda)\beta\big)^{-1}\gamma(\lambda)^*(A_{[\beta]} - \lambda)^{-k} \in \mathfrak{S}_p\big(L^2(\mathbb{R}^n_+), L^2(\partial\mathbb{R}^n_+)\big),$$
$$(A_{[\beta]} - \lambda)^{-k}\gamma(\lambda)\big(I - \beta M(\lambda)\big)^{-1}\alpha \in \mathfrak{S}_p\big(L^2(\partial\mathbb{R}^n_+), L^2(\mathbb{R}^n_+)\big).$$

Proof. Let us fix $\lambda_0 < -\|\beta\|^2_\infty$. Lemma 5.13 and the assumption on β imply that for $k = 0, 1, 2, \ldots, m-1$

$$\operatorname{ran}\big((A_{[\beta]} - \lambda_0)^{-k}\big) \subset H^{2k}(\mathbb{R}^n_+).$$

Further, we apply Lemma 4.15 and get

$$\operatorname{ran}\big(\big(I - M(\lambda_0)\beta\big)^{-1}\gamma(\lambda_0)^*(A_{[\beta]} - \lambda_0)^{-k}\big) \subset H^{2k+3/2}(\partial\mathbb{R}^n_+).$$

The items of this proposition follow from the corresponding items of Lemma 2.25 with $s = 2k + 3/2$. □

5.3.3 Resolvent power differences in $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$-classes and trace formulae

In the following two main theorems of this chapter we provide $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$-properties of the resolvent power differences of the self-adjoint Robin Laplacians $A_{[\beta_1]}$ and $A_{[\beta_2]}$ on the half-space. For these results smoothness of β_1 and β_2, and decay of $\beta_1 - \beta_2$ are important. In the proofs the key idea consists in factorizing $|\beta|$ in a proper way.

Theorem 5.15. *Let $\beta_1, \beta_2 \in W^{2m-1,\infty}(\partial\mathbb{R}^n_+)$ be real-valued, and denote $\beta := \beta_2 - \beta_1$. Let $A_{[\beta_1]}$ and $A_{[\beta_2]}$ be the self-adjoint Robin Laplacians on the half-space corresponding via (5.3.1) to β_1 and β_2, respectively. Assume that $l \in [1, m] \cap \mathbb{N}$ is arbitrary.*

(i) *If at least one of these two conditions:*

  (a) *β is compactly supported;*

(b) *$n > 4l$ and $\beta \in L^{\frac{n-1}{2l+1}}(\partial\mathbb{R}^n_+)$;*

holds, then

$$(A_{[\beta_2]} - \lambda)^{-l} - (A_{[\beta_1]} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n_+)\big) \tag{5.3.12}$$

for all $\lambda \in \rho(A_{[\beta_1]}) \cap \rho(A_{[\beta_2]})$.

(ii) *If $m > \frac{n}{2} - 1$, $l \in \mathbb{N}$ such that $\frac{n}{2} - 1 < l \leq m$, and at least one of the conditions (a) or (b) in item (i) holds, then for all $\lambda \in \rho(A_{[\beta_1]}) \cap \rho(A_{[\beta_2]})$ the operator in (5.3.12) belongs to the trace class, and the following formula*

$$\begin{aligned}\operatorname{tr}&\Big((A_{[\beta_2]} - \lambda)^{-l} - (A_{[\beta_1]} - \lambda)^{-l}\Big)\\ &= \frac{1}{(l-1)!}\operatorname{tr}\left(\frac{d^{l-1}}{d\lambda^{l-1}}\Big(U(\lambda)M'(\lambda)\Big)\right)\end{aligned}$$

holds, where $U(\lambda) := \big(I - \beta_2 M(\lambda)\big)^{-1}\beta\big(I - M(\lambda)\beta_1\big)^{-1}$.

Proof. (i) Let us fix $\lambda_0 < -\max\{\|\beta_1\|^2_\infty, \|\beta_2\|^2_\infty\}$. By Theorem 5.5 the resolvent difference of the self-adjoint operators $A_{[\beta_1]}$ and $A_{[\beta_2]}$ can be expressed as

$$\begin{aligned}&(A_{[\beta_2]} - \lambda_0)^{-1} - (A_{[\beta_1]} - \lambda_0)^{-1}\\ &\qquad = \gamma(\lambda_0)\big(I - \beta_2 M(\lambda_0)\big)^{-1}\beta\big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^*.\end{aligned} \tag{5.3.13}$$

For all $s \in [0,1]$, we define the operators

$$\begin{aligned}F_s(\lambda_0) &:= \gamma(\lambda_0)\big(I - \beta_2 M(\lambda_0)\big)^{-1}|\beta|^s,\\ G_s(\lambda_0) &:= \operatorname{sign}(\beta)|\beta|^s\big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^*.\end{aligned}$$

Observe that for each $s \in [0,1]$ the resolvent difference in (5.3.13) can be rewritten

$$(A_{[\beta_2]} - \lambda_0)^{-1} - (A_{[\beta_1]} - \lambda_0)^{-1} = F_{1-s}(\lambda_0)G_s(\lambda_0).$$

Denote $s(k) := \frac{2k+3/2}{2l+1}$ for $k = 0,1,2,\ldots,l-1$. Hence, the operators $T_{l,k}(\lambda_0)$ as in (2.1.2) with $H = A_{[\beta_1]}$ and $K = A_{[\beta_2]}$ can be represented as

$$T_{l,k}(\lambda_0) = (A_{[\beta_2]} - \lambda_0)^{-(l-k-1)}F_{1-s(k)}\lambda_0) \cdot G_{s(k)}(\lambda_0)(A_{[\beta_1]} - \lambda_0)^{-k}.$$

If β is compactly supported (condition (a) holds), then also $|\beta|^{1-s(k)}$ and $\operatorname{sign}(\beta)|\beta|^{s(k)}$ are compactly supported. Hence Proposition 5.14 (i) and Lemma 2.3 yield

$$
\begin{aligned}
&(A_{[\beta_2]} - \lambda_0)^{-(l-k-1)} F_{1-s(k)}(\lambda_0) \in \mathfrak{S}_{\frac{n-1}{2l-2k-1/2},\infty},\\
&G_{s(k)}(\lambda_0)(A_{[\beta_1]} - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}.
\end{aligned}
\tag{5.3.14}
$$

If β is such that condition (b) holds, then for all $k = 0, 1, 2 \ldots, l-1$ we obtain

$$
|\beta|^{1-s(k)} \in L^{\frac{n-1}{2l-2k-1/2}}(\partial\mathbb{R}^n_+) \quad \text{and} \quad \operatorname{sign}(\beta)|\beta|^{s(k)} \in L^{\frac{n-1}{2k+3/2}}(\partial\mathbb{R}^n_+).
$$

Note that under assumption $n > 4l$ we have

$$
\frac{n-1}{2l-2k-1/2} > 2 \quad \text{and} \quad \frac{n-1}{2k+3/2} > 2
$$

for all $k = 0, 1, 2, \ldots, l-1$. Proposition 5.14 (i) and Lemma 2.3 yield

$$
\begin{aligned}
&(A_{[\beta_2]} - \lambda_0)^{-(l-k-1)} F_{1-s(k)}(\lambda_0) \in \mathfrak{S}_{\frac{n-1}{2l-2k-1/2},\infty},\\
&G_{s(k)}(\lambda_0)(A_{[\beta_1]} - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty}.
\end{aligned}
\tag{5.3.15}
$$

Now we can conclude from (5.3.14) in the case, that condition (a) holds, and from (5.3.15) in the case, that condition (b) holds, that

$$
T_{l,k}(\lambda_0) \in \mathfrak{S}_{\frac{n-1}{2l-2k-1/2},\infty} \cdot \mathfrak{S}_{\frac{n-1}{2k+3/2},\infty} = \mathfrak{S}_{\frac{n-1}{2l+1},\infty}.
$$

for all $k = 0, 1, 2, \ldots, l-1$. Finally, Lemma 2.4 implies the statement.

(ii) The trace formula can be proved as in Theorem 3.17 (ii) with certain modifications, which are not explained in order to avoid repetitions. □

Corollary 5.16. *If, under the assumptions of the last theorem, β is compactly supported and $m > \frac{n}{2} - 1$, then the wave operators $W_\pm(A_{[\beta_1]}, A_{[\beta_2]})$ for the scattering pair $\{A_{[\beta_1]}, A_{[\beta_2]}\}$ exist and are complete. Hence, the absolutely continuous parts of $A_{[\beta_1]}$ and $A_{[\beta_2]}$ are unitarily equivalent.*

In the next theorem we consider the special case of an integrable difference of the Robin coefficients.

Theorem 5.17. *Assume that $n = 2$ or $n = 3$ holds. Let $\beta_1, \beta_2 \in W^{1,\infty}(\partial\mathbb{R}^n_+)$ be real-valued, and assume that $\beta := \beta_2 - \beta_1 \in L^1(\partial\mathbb{R}^n_+)$ holds. Let $A_{[\beta_1]}$ and $A_{[\beta_2]}$ be the self-adjoint Robin Laplacians on the half-space corresponding via (5.3.1) to β_1 and β_2, respectively. Then the property*

$$(A_{[\beta_2]} - \lambda)^{-1} - (A_{[\beta_1]} - \lambda)^{-1} \in \mathfrak{S}_1\big(L^2(\mathbb{R}^n_+)\big) \tag{5.3.16}$$

holds for all $\lambda \in \rho(A_{[\beta_1]}) \cap \rho(A_{[\beta_2]})$, and the trace of the resolvent difference in (5.3.16) can be expressed as

$$\operatorname{tr}\Big((A_{[\beta_2]} - \lambda)^{-1} - (A_{[\beta_1]} - \lambda)^{-1}\Big) = \operatorname{tr}\Big(U(\lambda)M'(\lambda)\Big),$$

where $U(\lambda) := \big(I - \beta_2 M(\lambda)\big)^{-1}\beta\big(I - M(\lambda)\beta_1\big)^{-1}$.

Proof. Let us fix $\lambda_0 < -\max\{\|\beta_1\|^2_\infty, \|\beta_2\|^2_\infty\}$. Observe that

$$\sqrt{|\beta|}, \sqrt{|\beta|}\operatorname{sign}(\beta) \in L^2(\mathbb{R}^{n-1}).$$

Note that for $n = 2$ or $n = 3$ the inequality $\frac{2(n-1)}{3} < 2$ holds. Hence, by Proposition 5.14 (ii)

$$\begin{aligned} &\sqrt{|\beta|}\big(I - M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^* \in \mathfrak{S}_2,\\ &\gamma(\lambda_0)\big(I - \beta_2 M(\lambda_0)\big)^{-1}\sqrt{|\beta|}\operatorname{sign}(\beta) \in \mathfrak{S}_2. \end{aligned} \tag{5.3.17}$$

By Theorem 5.5 the resolvent difference of self-adjoint operators $A_{[\beta_1]}$ and $A_{[\beta_2]}$ can be expressed as

$$(A_{[\beta_2]}-\lambda_0)^{-1}-(A_{[\beta_1]}-\lambda_0)^{-1} = \gamma(\lambda_0)\big(I-\beta_2 M(\lambda_0)\big)^{-1}\beta\big(I-M(\lambda_0)\beta_1\big)^{-1}\gamma(\lambda_0)^*.$$

In view of this factorization and of (5.3.17) we get

$$(A_{[\beta_2]} - \lambda_0)^{-1} - (A_{[\beta_1]} - \lambda_0)^{-1} \in \mathfrak{S}_2 \cdot \mathfrak{S}_2 = \mathfrak{S}_1.$$

Using Lemma 2.4 we conclude that

$$(A_{[\beta_2]} - \lambda)^{-1} - (A_{[\beta_1]} - \lambda)^{-1} \in \mathfrak{S}_1$$

for all $\lambda \in \rho(A_{[\beta_1]}) \cap \rho(A_{[\beta_2]})$.

The trace formula can be proven as in Theorem 3.17 (ii). $\square$

Corollary 5.18. *Under the assumptions of the last theorem, the wave operators $W_\pm(A_{[\beta_1]}, A_{[\beta_2]})$ for the scattering pair $\{A_{[\beta_1]}, A_{[\beta_2]}\}$ exist and are complete. Hence, the absolutely continuous parts of $A_{[\beta_1]}$ and $A_{[\beta_2]}$ are unitarily equivalent.*

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