Schrödinger Operators with δ and δ'-Potentials Supported on Hypersurfaces

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Abstract. Self-adjoint Schrödinger operators with δ and δ'-potentials supported on a smooth compact hypersurface are defined explicitly via boundary conditions. The spectral properties of these operators are investigated, regularity results on the functions in their domains are obtained, and analogues of the Birman–Schwinger principle and a variant of Krein's formula are shown. Furthermore, Schatten–von Neumann type estimates for the differences of the powers of the resolvents of the Schrödinger operators with δ and δ'-potentials, and the Schrödinger operator without a singular interaction are proved. An immediate consequence of these estimates is the existence and completeness of the wave operators of the corresponding scattering systems, as well as the unitary equivalence of the absolutely continuous parts of the singularly perturbed and unperturbed Schrödinger operators. In the proofs of our main theorems we make use of abstract methods from extension theory of symmetric operators, some algebraic considerations and results on elliptic regularity.

1. Introduction

Schrödinger operators with δ and δ'-potentials supported on hypersurfaces play an important role in mathematical physics and have attracted a lot of attention in the recent past; they are used for the description of quantum particles interacting with charged hypersurfaces. In this introduction we first define the differential operators which are studied in the present paper. Furthermore, we state and explain our main results on the spectral and scattering properties of these operators in an easily understandable but mathematically exact form in Theorems A–D below. Although the remaining part of the paper can be viewed as a proof of these theorems we mention that Sects. 3 and 4 contain not only slightly generalized versions of Theorems A–D but also other results which are of independent interest.

In the following let Σ be a compact connected C^∞-hypersurface which separates the Euclidean space $\mathbb{R}^n$ into a bounded domain Ω_i and an unbounded domain Ω_e with common boundary $\partial\Omega_e = \partial\Omega_i = \Sigma$. Denote by δ_Σ the δ-distribution supported on Σ and by δ'_Σ its normal derivative in the distributional sense with the normal pointing outwards of Ω_i. The main objective of the present paper is to define and study the spectral properties of Schrödinger operators associated with the formal differential expressions

$$\mathcal{L}_{\delta,\alpha} := -\Delta + V - \alpha \left\langle \delta_\Sigma, \cdot \right\rangle \delta_\Sigma \quad \text{and} \quad \mathcal{L}_{\delta',\beta} := -\Delta + V - \beta \left\langle \delta'_\Sigma, \cdot \right\rangle \delta'_\Sigma. \quad (1.1)$$

Here $V \in L^\infty(\mathbb{R}^n)$ is assumed to be a real-valued potential and $\alpha, \beta : \Sigma \to \mathbb{R}$ are real-valued measurable functions, often called strengths of interactions in mathematical physics. In order to define the Schrödinger operators with δ and δ'-interactions rigorously, it is necessary to specify suitable domains in $L^2(\mathbb{R}^n)$ which take into account the δ and δ'-interaction on the hypersurface Σ. In our approach this will be done explicitly via suitable interface conditions on Σ for a certain function space in $L^2(\mathbb{R}^n)$. One of the main advantages of our method compared with the usual approach via semi-bounded closed sesquilinear forms (see, e.g. [18,30]) is that δ'-interactions can be treated without any additional difficulties.

Throughout the paper we write the functions $f \in L^2(\mathbb{R}^n)$ in the form $f = f_i \oplus f_e$ with respect to the corresponding space decomposition $L^2(\Omega_i) \oplus L^2(\Omega_e)$. For the definition of Schrödinger operators with δ or δ'-potentials we introduce the following subspaces

$$H_\Delta^{3/2}(\Omega_i) := \left\{ f_i \in H^{3/2}(\Omega_i) : \Delta f_i \in L^2(\Omega_i) \right\},$$
$$H_\Delta^{3/2}(\Omega_e) := \left\{ f_e \in H^{3/2}(\Omega_e) : \Delta f_e \in L^2(\Omega_e) \right\},$$

of the Sobolev spaces $H^{3/2}(\Omega_i)$ and $H^{3/2}(\Omega_e)$, respectively, and their orthogonal sum in $L^2(\mathbb{R}^n)$:

$$H_\Delta^{3/2}(\mathbb{R}^n \backslash \Sigma) := H_\Delta^{3/2}(\Omega_i) \oplus H_\Delta^{3/2}(\Omega_e);$$

cf. [2,59] and Sects. 2.3 and 2.4 for more details. The trace of a function $f_i \in H_\Delta^{3/2}(\Omega_i)$ and the trace of the normal derivative $\partial_{\nu_i} f_i$ (with the normal ν_i pointing outwards) are denoted by $f_i|_\Sigma$ and $\partial_{\nu_i} f_i|_\Sigma$, respectively. Similarly, for the exterior domain and $f_e \in H_\Delta^{3/2}(\Omega_e)$ we write $f_e|_\Sigma$ and $\partial_{\nu_e} f_e|_\Sigma$; here ν_e and ν_i are pointing in opposite directions.

The main objects we study in this paper are the operators given in the following definition, which are associated with the formal differential expressions in (1.1).

Definition. Let $\alpha \in L^\infty(\Sigma)$ be a real-valued function on Σ. The Schrödinger operator $A_{\delta,\alpha}$ corresponding to the δ-interaction with strength α on Σ is defined as

$$A_{\delta,\alpha} f := -\Delta f + V f,$$

$$\operatorname{dom} A_{\delta,\alpha} := \left\{ f \in H_\Delta^{3/2}(\mathbb{R}^n \backslash \Sigma) : \begin{array}{c} f_i|_\Sigma = f_e|_\Sigma \\ \alpha f_i|_\Sigma = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma \end{array} \right\}.$$

Let β be a real-valued function on Σ such that $1/\beta \in L^\infty(\Sigma)$. The Schrödinger operator $A_{\delta',\beta}$ corresponding to the δ'-interaction with strength β on Σ is defined as

$$A_{\delta',\beta} f := -\Delta f + V f,$$

$$\operatorname{dom} A_{\delta',\beta} := \left\{ f \in H^{3/2}_\Delta(\mathbb{R}^n \backslash \Sigma) : \begin{array}{l} \partial_{\nu_e} f_e|_\Sigma = -\partial_{\nu_i} f_i|_\Sigma \\ \beta \partial_{\nu_e} f_e|_\Sigma = f_e|_\Sigma - f_i|_\Sigma \end{array} \right\}.$$

The boundary conditions in the domains of $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ fit with the formal differential expressions in (1.1). In order to see this for $A_{\delta,\alpha}$ we introduce the closed symmetric form

$$\mathfrak{a}_{\delta,\alpha}[f,g] = (\nabla f, \nabla g)_{L^2(\mathbb{R}^n;\mathbb{C}^n)} + (V f, g)_{L^2(\mathbb{R}^n)} - (\alpha f|_\Sigma, g|_\Sigma)_{L^2(\Sigma)}$$

on $H^1(\mathbb{R}^n)$. Further making use of the boundary conditions $f_i|_\Sigma = f_e|_\Sigma$ and $\alpha f_i|_\Sigma = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma$ for $f \in \operatorname{dom} A_{\delta,\alpha}$ and the first Green's identity one can easily see that

$$(A_{\delta,\alpha} f, g)_{L^2(\mathbb{R}^n)} = \mathfrak{a}_{\delta,\alpha}[f,g] = \langle \mathcal{L}_{\delta,\alpha} f, g \rangle$$

for all $g \in H^1(\mathbb{R}^n)$. This also shows that $A_{\delta,\alpha}$ coincides with the self-adjoint operator associated with the closed symmetric form $\mathfrak{a}_{\delta,\alpha}$; cf. Proposition 3.7 for more details. The quadratic form method has been used in various papers for the definition of Schrödinger operators with δ-perturbations supported on curves and hypersurfaces. We refer the reader to [18] and the review paper [30] for more details and further references; we also mention [19,28,29,32–35,39,58] for studies of eigenvalues, [16,31,38,70] for results on the absolutely continuous spectrum, and [6,36,37,40,41,54,60,67] for related problems for Schrödinger operators with δ-perturbations. We point out that the quadratic form approach could not be adapted to the δ'-case so far; see the open problem posed in [30, 7.2] and our solution in Proposition 3.15. For completeness we also mention that the above definitions of the differential operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ are compatible with the ones for one-dimensional δ and δ'-point interactions in [3,4].

In the next theorem, which is the first main result of this paper, we obtain some basic properties of the Schrödinger operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$. Here also the *free* or *unperturbed* Schrödinger operator

$$A_{\mathrm{free}} f = -\Delta f + V f, \qquad \operatorname{dom} A_{\mathrm{free}} = H^2(\mathbb{R}^n),$$

is used. It is well known and easy to see that A_{free} is semi-bounded and self-adjoint in $L^2(\mathbb{R}^n)$. Recall that the essential spectrum $\sigma_{\mathrm{ess}}(A)$ of a self-adjoint operator A consists of all spectral points that are not isolated eigenvalues of finite multiplicity. The statements in Theorem A below are contained in Theorems 3.5, 3.11, 3.14 and 3.16 in Sects. 3.2–3.4.

Theorem A. *The Schrödinger operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ are self-adjoint operators in $L^2(\mathbb{R}^n)$, which are bounded from below, and their essential spectra satisfy*

$$\sigma_{\mathrm{ess}}(A_{\delta,\alpha}) = \sigma_{\mathrm{ess}}(A_{\delta',\beta}) = \sigma_{\mathrm{ess}}(A_{\mathrm{free}}). \tag{1.2}$$

If $V \equiv 0$, then $\sigma_{\mathrm{ess}}(A_{\delta,\alpha}) = \sigma_{\mathrm{ess}}(A_{\delta',\beta}) = [0, \infty)$ and the negative spectra of the self-adjoint operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ consist of finitely many negative eigenvalues with finite multiplicities.

It is not surprising that additional smoothness assumptions on the functions α and β in the boundary condition yield more regularity for the functions in dom $A_{\delta,\alpha}$ and dom $A_{\delta',\beta}$. The H^2-case is of particular importance; see also [17] where the Laplacian on a strip was considered. The next theorem follows from Theorems 3.6 and 3.12. The Sobolev space of order one of L^∞-functions on Σ is denoted by $W^{1,\infty}(\Sigma)$.

Theorem B. *If $\alpha \in W^{1,\infty}(\Sigma)$, then dom $A_{\delta,\alpha}$ is contained in $H^2(\Omega_{\mathrm{i}}) \oplus H^2(\Omega_{\mathrm{e}})$. If $1/\beta \in W^{1,\infty}(\Sigma)$, then dom $A_{\delta',\beta}$ is contained in $H^2(\Omega_{\mathrm{i}}) \oplus H^2(\Omega_{\mathrm{e}})$.*

The fact that the essential spectra of the operators $A_{\delta,\alpha}$, $A_{\delta',\beta}$ and A_{free} in Theorem A coincide, follows from the observation that the resolvent differences of these operators are compact. Roughly speaking this is a consequence of the compactness of the hypersurface Σ and Sobolev embedding theorems. However, as can be expected from the classical results in [12] (see also [10,13,14, 23,49,52,53,61]), more specific considerations yield more precise Schatten–von Neumann type estimates for the differences of the resolvents and their integer powers, which then in turn imply existence and completeness of the wave operators of the scattering pairs $\{A_{\delta,\alpha}, A_{\mathrm{free}}\}$ and $\{A_{\delta',\beta}, A_{\mathrm{free}}\}$; see, e.g. [56,65,72] for more details and consequences.

Recall that a compact operator T is said to belong to the weak Schatten–von Neumann ideal $\mathfrak{S}_{p,\infty}$ if the sequence of singular values s_k, i.e. the sequence of eigenvalues of the non-negative operator $(T^*T)^{1/2}$, satisfies $s_k = O(k^{-1/p})$, $k \to \infty$. Note that $\mathfrak{S}_{p,\infty} \subset \mathfrak{S}_{p'}$ for all $p' > p$, where $\mathfrak{S}_{p'}$ is the usual Schatten–von Neumann ideal; cf. Sect. 2.1.

Theorem C. *For the self-adjoint Schrödinger operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ in $L^2(\mathbb{R}^n)$ the following statements hold.*

(i) *For all $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\mathrm{free}})$ we have*

$$(A_{\delta,\alpha} - \lambda)^{-1} - (A_{\mathrm{free}} - \lambda)^{-1} \in \mathfrak{S}_{\frac{n-1}{3},\infty}$$

and, in particular, the wave operators for the pair $\{A_{\delta,\alpha}, A_{\mathrm{free}}\}$ exist and are complete when $n = 2$ or $n = 3$.

(ii) *For all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{free}})$ we have*

$$(A_{\delta',\beta} - \lambda)^{-1} - (A_{\mathrm{free}} - \lambda)^{-1} \in \mathfrak{S}_{\frac{n-1}{2},\infty},$$

and, in particular, the wave operators for the pair $\{A_{\delta',\beta}, A_{\mathrm{free}}\}$ exist and are complete when $n = 2$.

The scattering theory for operators with δ-potentials in the two-dimensional case is partially developed in [36]. In higher dimensions it is necessary to extend the estimates to higher powers of resolvents as we do in the next main theorem under an additional local regularity assumption on the potential V. In particular, for sufficiently smooth V this implies the existence and

completeness of the wave operators for the scattering pairs $\{A_{\delta,\alpha}, A_{\text{free}}\}$ and $\{A_{\delta',\beta}, A_{\text{free}}\}$ in any space dimension. For $k \in \mathbb{N}_0$ the subspace of $L^\infty(\mathbb{R}^n)$ which consists of all functions that admit partial derivatives in an open neighbourhood of the hypersurface Σ up to order k in $L^\infty(\mathbb{R}^n)$ is denoted by $W_\Sigma^{k,\infty}(\mathbb{R}^n)$.

Theorem D. *Let the self-adjoint Schrödinger operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ be as above, and assume that $V \in W_\Sigma^{2m-2,\infty}(\mathbb{R}^n)$ for some $m \in \mathbb{N}$. Then the following statements hold.*

(i) *For all $l = 1, 2, \ldots, m$ and $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\text{free}})$ we have*

$$(A_{\delta,\alpha} - \lambda)^{-l} - (A_{\text{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty},$$

and, in particular, the wave operators for the pair $\{A_{\delta,\alpha}, A_{\text{free}}\}$ exist and are complete when $2m - 2 > n - 4$.

(ii) *For all $l = 1, 2, \ldots, m$ and $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{free}})$ we have*

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\text{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty},$$

and, in particular, the wave operators for the pair $\{A_{\delta',\beta}, A_{\text{free}}\}$ exist and are complete when $2m - 2 > n - 3$.

Note that, for $m = 1$, Theorem D reduces to Theorem C. The proof of Theorem D is essentially a consequence of Krein's formula, some algebraic considerations and results on elliptic regularity. The statements in Theorem D are contained in Theorems 4.3, 4.5 and Corollaries 4.4, 4.7.

The paper is organized as follows. Section 2 contains preliminary material on Schatten–von Neumann classes, general extension theory of symmetric operators and function spaces. In particular, we prove some useful abstract lemmas on resolvent power differences in Sect. 2.1. Furthermore, in Sect. 2.2 we collect basic facts about quasi boundary triples—a convenient abstract tool from [8,9] to study self-adjoint extensions of symmetric partial differential operators—and recall a variant of Krein's formula suitable for our purposes. Section 3 is devoted to the rigorous mathematical definition and the investigation of the spectral properties of the operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$. In Sects. 3.2 and 3.3 we provide proofs of self-adjointness and sufficient conditions for H^2-regularity of the operator domains, cf. Theorems A and B, and we discuss variants of the Birman–Schwinger principle for the description of eigenvalues of the self-adjoint operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$. All these results are obtained by means of suitable quasi boundary triples constructed in these sections. Section 3.2 is accompanied by a comparison with the sesquilinear form approach to Schrödinger operators with δ-potentials on hypersurfaces. In Sect. 3.4 we obtain basic spectral properties of the self-adjoint operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ such as lower semi-boundedness and finiteness of negative spectra if $V \equiv 0$. Section 4 contains our main results on Schatten–von Neumann estimates from Theorems C and D for resolvent power differences of operators $A_{\delta,\alpha}, A_{\delta',\beta}$ and A_{free}. As a direct consequence of these estimates we establish the existence and completeness of wave operators for certain scattering pairs arising in quantum mechanics.

We emphasize again that the results in the body of the paper are sometimes stronger than in the introduction. Several theorems of their own independent interest are formulated only in the main part. We also mention that many of the results in the paper extend to more general second order differential operators with sufficiently smooth coefficients and also remain to be true under weaker assumptions on the smoothness of the hypersurface Σ; in this context we refer the reader to the recent papers [1,7,43–46,63] on elliptic operators in non-smooth domains.

2. Preliminaries

This section contains some preliminary material that will be used in the main part of the paper. In Sect. 2.1 we first recall some basic properties of Schatten–von Neumann ideals and we prove an abstract lemma with sufficient conditions for resolvent power differences to belong to some Schatten–von Neumann class. The concept of quasi boundary triples and their Weyl functions from general extension theory of symmetric operators is briefly reviewed in Sect. 2.2. Sections 2.3 and 2.4 contain mainly definitions and notations for the function spaces used in the paper.

2.1. $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$-Classes

Let $\mathcal{H}$ and $\mathcal{G}$ be separable Hilbert spaces. The space of bounded everywhere defined linear operators from $\mathcal{H}$ into $\mathcal{G}$ is denoted by $\mathcal{B}(\mathcal{H},\mathcal{G})$, and we set $\mathcal{B}(\mathcal{H}) := \mathcal{B}(\mathcal{H},\mathcal{H})$. The ideal of compact operators mapping from $\mathcal{H}$ into $\mathcal{G}$ is denoted by $\mathfrak{S}_\infty(\mathcal{H},\mathcal{G})$, and we set $\mathfrak{S}_\infty(\mathcal{H}) := \mathfrak{S}_\infty(\mathcal{H},\mathcal{H})$. We agree to write $\mathfrak{S}_\infty$ when it is clear from the context between which spaces the operators act. The *singular values* (or *s-numbers*) $s_k(T), k = 1, 2, \ldots$, of a compact operator $T \in \mathfrak{S}_\infty(\mathcal{H},\mathcal{G})$ are defined as the eigenvalues of the non-negative compact operator $(T^*T)^{1/2}$, enumerated in non-increasing order and with multiplicities taken into account. Recall that the singular values of T and T^* coincide; see, e.g. [47, II.§2.2]. The Schatten–von Neumann class of operator ideals $\mathfrak{S}_p$ and the weak Schatten–von Neumann class of operator ideals $\mathfrak{S}_{p,\infty}$ are defined as

$$\mathfrak{S}_p := \left\{ T \in \mathfrak{S}_\infty \colon \sum_{k=1}^{\infty} \big(s_k(T)\big)^p < \infty \right\}, \qquad p > 0;$$
$$\mathfrak{S}_{p,\infty} := \left\{ T \in \mathfrak{S}_\infty \colon s_k(T) = O(k^{-1/p}),\ k \to \infty \right\},$$

they play an important role later on. We refer the reader to [47, III.§7 and III.§14], [69, Chapter 2] and to [15, Chapter 11] for a detailed study of the classes $\mathfrak{S}_p$ and $\mathfrak{S}_{p,\infty}$. If a compact operator $T \in \mathfrak{S}_\infty(\mathcal{H},\mathcal{G})$ belongs to $\mathfrak{S}_p$ or $\mathfrak{S}_{p,\infty}$, then we also write $T \in \mathfrak{S}_p(\mathcal{H},\mathcal{G})$ or $T \in \mathfrak{S}_{p,\infty}(\mathcal{H},\mathcal{G})$, respectively, if the spaces $\mathcal{H}$ and $\mathcal{G}$ are important in the context. Moreover, we set

$$\mathfrak{S}_p \cdot \mathfrak{S}_q := \big\{ T_1 T_2 \colon T_1 \in \mathfrak{S}_p, T_2 \in \mathfrak{S}_q \big\},$$

$$\mathfrak{S}_{p,\infty} \cdot \mathfrak{S}_{q,\infty} := \big\{ T_1 T_2 \colon T_1 \in \mathfrak{S}_{p,\infty}, T_2 \in \mathfrak{S}_{q,\infty} \big\}.$$

The proof of the next statement can be found in [15,47] and, e.g. [11, Lemma 2.3].

Lemma 2.1. *Let $p, q, r, s, t > 0$. Then the following statements are true:*

(i) $\mathfrak{S}_p \cdot \mathfrak{S}_q = \mathfrak{S}_r$ *and* $\mathfrak{S}_{p,\infty} \cdot \mathfrak{S}_{q,\infty} = \mathfrak{S}_{r,\infty}$ *when* $p^{-1} + q^{-1} = r^{-1}$, *or, equivalently*

$$\mathfrak{S}_{\frac{1}{s}} \cdot \mathfrak{S}_{\frac{1}{t}} = \mathfrak{S}_{\frac{1}{s+t}} \qquad and \qquad \mathfrak{S}_{\frac{1}{s},\infty} \cdot \mathfrak{S}_{\frac{1}{t},\infty} = \mathfrak{S}_{\frac{1}{s+t},\infty};$$

(ii) *If $T \in \mathfrak{S}_p$, then $T^* \in \mathfrak{S}_p$; if $T \in \mathfrak{S}_{p,\infty}$, then $T^* \in \mathfrak{S}_{p,\infty}$;*

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

Let H and K be linear operators in a separable Hilbert space $\mathcal{H}$ and assume that $\rho(H) \cap \rho(K) \neq \varnothing$. In order to investigate properties of the difference of the mth powers of the resolvents,

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

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

$$a^m - b^m = \sum_{k=0}^{m-1} a^{m-k-1}(a-b)b^k. \tag{2.1}$$

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

$$T_{m,k}(\lambda) := (H - \lambda)^{-(m-k-1)}\left((H-\lambda)^{-1} - (K-\lambda)^{-1}\right)(K-\lambda)^{-k} \tag{2.2}$$

for $\lambda \in \rho(H) \cap \rho(K), m \in \mathbb{N}$ and $k = 0, 1, \ldots, m-1$, we conclude from (2.1) that

$$(H - \lambda)^{-m} - (K - \lambda)^{-m} = \sum_{k=0}^{m-1} T_{m,k}(\lambda) \tag{2.3}$$

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 $\mathfrak{S}_{p,\infty}$ for all $\lambda \in \rho(H) \cap \rho(K)$ if all the operators $T_{m,0}(\lambda_0), T_{m,1}(\lambda_0), \ldots, T_{m,m-1}(\lambda_0)$ belong to $\mathfrak{S}_{p,\infty}$ for some $\lambda_0 \in \rho(H) \cap \rho(K)$. In the case $m = 1$ the statement is well known. We note that the statement holds in the same form if the class $\mathfrak{S}_{p,\infty}$ is replaced by any operator ideal, e.g. $\mathfrak{S}_p$.

Lemma 2.2. *Let H and K be linear operators in $\mathcal{H}$ such that $\rho(H) \cap \rho(K) \neq \varnothing$. Moreover, let $p > 0, m \in \mathbb{N}$ and $T_{m,k}$ be as in (2.2), and assume that $T_{m,k}(\lambda_0) \in \mathfrak{S}_{p,\infty}(\mathcal{H})$ for some $\lambda_0 \in \rho(H) \cap \rho(K)$ and all $k = 0, 1, \ldots, m-1$. Then*

$$(H - \lambda)^{-m} - (K - \lambda)^{-m} \in \mathfrak{S}_{p,\infty}(\mathcal{H})$$

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

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

$$E_\lambda := I + (\lambda - \lambda_0)(H - \lambda)^{-1} \quad \text{and} \quad F_\lambda := I + (\lambda - \lambda_0)(K - \lambda)^{-1}. \tag{2.4}$$

The resolvent identity implies that

$$E_\lambda(H - \lambda_0)^{-1} = (H - \lambda_0)^{-1} + (\lambda - \lambda_0)(H - \lambda)^{-1}(H - \lambda_0)^{-1} = (H - \lambda)^{-1} \tag{2.5}$$

and, similarly,

$$(K - \lambda_0)^{-1} F_\lambda = (K - \lambda)^{-1}. \tag{2.6}$$

By induction we obtain

$$E_\lambda^l(H - \lambda_0)^{-l} = (H - \lambda)^{-l} \quad \text{and} \quad (K - \lambda_0)^{-l} F_\lambda^l = (K - \lambda)^{-l} \tag{2.7}$$

for all $l \in \mathbb{N}$. Set $D_1(\lambda) := (H - \lambda)^{-1} - (K - \lambda)^{-1}, \lambda \in \rho(H) \cap \rho(K)$. Then (2.5), (2.6) and (2.4) imply that

$$
\begin{aligned}
E_\lambda D_1(\lambda_0) F_\lambda &= E_\lambda(H - \lambda_0)^{-1} F_\lambda - E_\lambda(K - \lambda_0)^{-1} F_\lambda \\
&= (H - \lambda)^{-1} F_\lambda - E_\lambda(K - \lambda)^{-1} \\
&= (H - \lambda)^{-1} + (\lambda - \lambda_0)(H - \lambda)^{-1}(K - \lambda)^{-1} \\
&\quad -(K - \lambda)^{-1} - (\lambda - \lambda_0)(H - \lambda)^{-1}(K - \lambda)^{-1} \\
&= D_1(\lambda).
\end{aligned}
\tag{2.8}
$$

For $k = 0, 1 \ldots, m - 1$ and all $\lambda \in \rho(H) \cap \rho(K)$ we obtain from (2.7), (2.8) and the facts that E_λ commutes with $(H - \lambda_0)^{-1}$ and F_λ commutes with $(K - \lambda_0)^{-1}$ the following relation

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

By assumption, $T_{m,k}(\lambda_0) \in \mathfrak{S}_{p,\infty}$, and hence we conclude that $T_{m,k}(\lambda) \in \mathfrak{S}_{p,\infty}$ for $k = 0, 1, \ldots, m - 1$ and $\lambda \in \rho(H) \cap \rho(K)$. This together with (2.3) implies that

$$(H - \lambda)^{-m} - (K - \lambda)^{-m} = \sum_{k=0}^{m-1} T_{m,k}(\lambda) \in \mathfrak{S}_{p,\infty}(\mathcal{H})$$

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

The following lemma will be used in Sect. 4.2 to show that certain resolvent power differences are in some class $\mathfrak{S}_{p,\infty}$.

Lemma 2.3. *Let H and K be linear operators in $\mathcal{H}$, let $\mathcal{K}$ be an auxiliary Hilbert space and assume that, for some $\lambda_0 \in \rho(H) \cap \rho(K)$, there exist operators $B \in \mathcal{B}(\mathcal{K}, \mathcal{H})$ and $C \in \mathcal{B}(\mathcal{H}, \mathcal{K})$ such that*

$$(H - \lambda_0)^{-1} - (K - \lambda_0)^{-1} = BC. \tag{2.9}$$

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 $r \in \mathbb{N}$ and assume that

$$(K - \lambda_0)^{-k} B \in \mathfrak{S}_{\frac{1}{ak+b_1}, \infty},$$
$$C(K - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak+b_2}, \infty}, \qquad k = 0, 1, \ldots, r - 1. \tag{2.10}$$

Then

$$(H - \lambda)^{-l} - (K - \lambda)^{-l} \in \mathfrak{S}_{\frac{1}{al+b}, \infty} \tag{2.11}$$

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

Proof. We prove the statement by induction with respect to l. Using the factorization in (2.9), the assumptions in (2.10) with $k = 0$ and Lemma 2.1 (i) we obtain

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

Now Lemma 2.2 with $m = 1$ implies that

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

for all $\lambda \in \rho(H) \cap \rho(K)$, i.e. (2.11) is true for $l = 1$.

For the induction step fix $m \in \mathbb{N}, 2 \leq m \leq r$ and assume that (2.11) is satisfied for all $l = 1, 2, \ldots, m - 1$. For $k = 0, 1, \ldots, m - 1$ let $T_{m,k}$ be as in (2.2), define

$$D_j(\lambda_0) := (H - \lambda_0)^{-j} - (K - \lambda_0)^{-j}, \qquad j \in \mathbb{N}_0,$$

and write

$$T_{m,k}(\lambda_0) = (H - \lambda_0)^{-(m-k-1)} BC(K - \lambda_0)^{-k}$$
$$= D_{m-k-1}(\lambda_0) BC(K - \lambda_0)^{-k}$$
$$+ (K - \lambda_0)^{-(m-k-1)} BC(K - \lambda_0)^{-k}. \tag{2.12}$$

Note that $D_0(\lambda_0) = 0$. By assumption (2.10) we have

$$B \in \mathfrak{S}_{\frac{1}{b_1}, \infty}, \quad C(K - \lambda_0)^{-k} \in \mathfrak{S}_{\frac{1}{ak+b_2}, \infty},$$
$$(K - \lambda_0)^{-(m-k-1)} B \in \mathfrak{S}_{\frac{1}{a(m-k-1)+b_1}, \infty},$$

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

$$D_{m-k-1}(\lambda_0) \in \mathfrak{S}_{\frac{1}{a(m-k-1)+b}, \infty}$$

for $k = 0, 1, \ldots, m - 1$, and and hence we obtain with Lemma 2.1 (i) that the first summand in (2.12) is in

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

where we used that $b \geq 0$. The second summand in (2.12) is in

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

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 (2.11) for $l = m$. $\qquad \square$

2.2. Quasi Boundary Triples and Their Weyl Functions

The concept of quasi boundary triples and Weyl functions is a generalization of the notion of (ordinary) boundary triples and Weyl functions from [20, 26, 48, 57], which is a very convenient tool in extension theory of symmetric operators. Quasi boundary triples are particularly useful when dealing with elliptic boundary value problems from an operator and extension theoretic point of view. In this subsection we provide some general facts on quasi boundary triples, which can be found in [8] and [9].

Throughout this subsection let $(\mathcal{H}, (\cdot, \cdot)_\mathcal{H})$ be a Hilbert space and let A be a densely defined closed symmetric operator in $\mathcal{H}$.

Definition 2.4. A triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called a *quasi boundary triple* for A^* if $(\mathcal{G}, (\cdot, \cdot)_\mathcal{G})$ 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 ran $\binom{\Gamma_0}{\Gamma_1}$ is dense 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* holds:

$$(Tf, g)_\mathcal{H} - (f, Tg)_\mathcal{H} = (\Gamma_1 f, \Gamma_0 g)_\mathcal{G} - (\Gamma_0 f, \Gamma_1 g)_\mathcal{G}. \qquad (2.13)$$

The following simple example illustrates the notion of quasi boundary triples for the Laplacian on a smooth bounded domain, see [8,9], Section 3.1 and Proposition 3.1.

Example. Let Ω be a bounded domain with smooth boundary, $A = -\Delta$ with $\operatorname{dom} A = H_0^2(\Omega), T = -\Delta$ with $\operatorname{dom} T = H^2(\Omega)$, let $\mathcal{G} = L^2(\partial\Omega)$ and define the boundary mappings as

$$\Gamma_0 f = \partial_\nu f|_{\partial\Omega}, \quad \Gamma_1 f = f|_{\partial\Omega}, \qquad f \in \operatorname{dom} T;$$

where ∂_ν stands for the normal derivative with normal vector pointing outwards. It can be shown that the closure of T coincides with the adjoint operator $A^* = -\Delta, \operatorname{dom} A^* = \{f \in L^2(\Omega) : \Delta f \in L^2(\Omega)\}$, and that the properties of (i)–(iii) in Definition 2.4 hold. Hence $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^*.

We remark that a quasi boundary triple for the adjoint A^* of a densely defined closed symmetric operator 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 $T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1)$ 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 [25, 27]. In the special case that the deficiency indices $n_\pm(A)$ of A are finite (and coincide) a quasi boundary triple is automatically an ordinary boundary triple.

The following proposition contains a sufficient condition for a triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ to be a quasi boundary triple, cf. [8, Theorem 2.3] and [9, Theorem 2.3]. The result will be applied in Sects. 3.2 and 3.3.

Proposition 2.5. *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) *The range of $\left(\begin{smallmatrix}\Gamma_0\\\Gamma_1\end{smallmatrix}\right) \colon \operatorname{dom} T \to \mathcal{G} \times \mathcal{G}$ is dense and $\ker\Gamma_0 \cap \ker\Gamma_1$ is dense in $\mathcal{H}$.*
(b) *The identity (2.13) holds for all $f, g \in \operatorname{dom} T$.*
(c) *$T \restriction \ker\Gamma_0$ is an extension of a self-adjoint operator A_0.*

Then $A := T \restriction \ker\Gamma_0 \cap \ker\Gamma_1$ is a densely defined closed symmetric operator in $\mathcal{H}$, and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for A^* with $A_0 = T \restriction \ker\Gamma_0$.

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

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

holds for all $\lambda \in \rho(A_0)$. Hence $\Gamma_0 \restriction \ker(T - \lambda)$ is invertible for all $\lambda \in \rho(A_0)$ and maps $\ker(T - \lambda)$ bijectively onto $\operatorname{ran}\Gamma_0$.

Definition 2.6. *Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = A^*$ and $A_0 = T \restriction \ker\Gamma_0$. Then the (operator-valued) functions γ and M defined by*

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

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

The values of the Weyl function corresponding to the quasi boundary triple $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$ in the example below Definition 2.4 are Neumann-to-Dirichlet maps; cf. [8,9], Sect. 3.1 and Proposition 3.1.

The definitions of γ and M 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, cf. [26]. 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

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda, \quad f_\lambda \in \ker(T - \lambda), \quad \lambda \in \rho(A_0).$$

In the next proposition we collect some properties of the γ-field and the Weyl function; all statements are proved in [8].

Proposition 2.7. *Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = A^*$ with $A_0 = T \restriction \ker\Gamma_0, \gamma$-field γ and Weyl function M. Then, for $\lambda \in \rho(A_0)$, the following assertions hold.*

(i) *The mapping $\gamma(\lambda)$ is a densely defined bounded operator from $\mathcal{G}$ into $\mathcal{H}$ with $\operatorname{dom}\gamma(\lambda) = \operatorname{ran}\Gamma_0$.*
(ii) *The adjoint of $\gamma(\overline{\lambda})$ satisfies*

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

(iii) *The values of the Weyl function M are densely defined (in general unbounded) operators in $\mathcal{G}$ with $\operatorname{dom} M(\lambda) = \operatorname{ran} \Gamma_0$ and $\operatorname{ran} M(\lambda) \subset \operatorname{ran} \Gamma_1$. Furthermore, $M(\overline{\lambda}) \subset M(\lambda)^*$ holds.*
(iv) *If $\operatorname{ran} \Gamma_0 = \mathcal{G}$, then $M(\lambda) \in \mathcal{B}(\mathcal{G})$.*
(v) *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 $M(\lambda)$ is a bijective mapping from $\operatorname{ran} \Gamma_0$ onto $\operatorname{ran} \Gamma_1$.*

With the help of a quasi boundary triple and the associated Weyl function it is possible to describe the spectral properties of extensions of A, which are restrictions of $T \subset A^*$. The extensions A_Θ are defined with the help of an abstract boundary condition by

$$A_\Theta := T \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0) = T \upharpoonright \ker(\Theta^{-1}\Gamma_1 - \Gamma_0), \tag{2.14}$$

where Θ is a linear operator in $\mathcal{G}$ or a linear relation in $\mathcal{G}$, i.e. a subspace of $\mathcal{G} \times \mathcal{G}$, cf. [8]. The sums and products are understood in the sense of linear relations if Θ or Θ^{-1} is not a (single-valued) operator. However, for our purposes the case that Θ^{-1} is a bounded linear operator on $\mathcal{G}$ is of particular interest and linear relations will not be used in the following. The next statement contains a variant of Krein's formula in this case; see [8, Theorem 2.8 and Theorem 4.8], [9, Theorem 3.7 and Corollary 3.9] and [11, Theorem 3.13].

Theorem 2.8. *Let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $\overline{T} = A^*$ with $A_0 = T \upharpoonright \ker \Gamma_0, \gamma$-field γ and Weyl function M. Furthermore, let $B = B^* = \Theta^{-1} \in \mathcal{B}(\mathcal{G})$ and let*

$$A_\Theta = T \upharpoonright \ker(B\Gamma_1 - \Gamma_0) \tag{2.15}$$

be the corresponding extension as in (2.14). Then, for $\lambda \in \rho(A_0)$, the following assertions hold.

(i) *$\lambda \in \sigma_p(A_\Theta)$ if and only if $\ker(I - BM(\lambda)) \neq \{0\}$. Moreover, in this case, the multiplicity of the eigenvalue λ of A_Θ is equal to $\dim \ker(I - BM(\lambda))$.*
(ii) *For all $g \in \operatorname{ran}(A_\Theta - \lambda)$ and $\lambda \notin \sigma_p(A_\Theta)$ we have*

$$(A_\Theta - \lambda)^{-1}g - (A_0 - \lambda)^{-1}g = \gamma(\lambda)(I - BM(\lambda))^{-1}B\gamma(\overline{\lambda})^*g.$$

If, in addition, $\operatorname{ran} \Gamma_0 = \mathcal{G}$ and $M(\lambda_0) \in \mathfrak{S}_\infty(\mathcal{G})$ for some $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$, then the operator A_Θ in (2.15) is self-adjoint in $\mathcal{H}$, Krein's formula

$$(A_\Theta - \lambda)^{-1} - (A_0 - \lambda)^{-1} = \gamma(\lambda)(I - BM(\lambda))^{-1}B\gamma(\overline{\lambda})^* \tag{2.16}$$

holds for all $\lambda \in \rho(A_\Theta) \cap \rho(A_0)$, and $(I - BM(\lambda))^{-1} \in \mathcal{B}(\mathcal{G})$.

2.3. Sobolev Spaces, Traces and Green's Identities

Throughout this paper Sobolev spaces and certain interpolation spaces play an important role. In this subsection we provide some necessary definitions and basic properties. The reader is referred, e.g. to the monographs [2,51,59,62] for more details.

Let $\Omega \subset \mathbb{R}^n$ be an arbitrary bounded or unbounded domain with a compact C^∞-boundary $\partial\Omega$. By $H^s(\Omega)$ and $H^s(\partial\Omega), s \in \mathbb{R}$, we denote the standard (L^2-based) Sobolev spaces of order s of functions in Ω and $\partial\Omega$, respectively. The inner product and norm on H^s are denoted by $(\cdot, \cdot)_s$ and $\| \cdot \|_s$, for $s = 0$

we simply write $(\cdot, \cdot)$ and $\|\cdot\|$, respectively. In order to avoid possible confusion, sometimes also the space is used as an index, e.g. $(\cdot, \cdot)_{L^2(\Omega)}$ and $(\cdot, \cdot)_{L^2(\partial\Omega)}$. The Sobolev spaces of order $k \in \mathbb{N}_0$ of L^∞-functions on Ω and $\partial\Omega$ are denoted by $W^{k,\infty}(\Omega)$ and $W^{k,\infty}(\partial\Omega)$, respectively. The following well-known implications will be used later:

$$\begin{aligned} f \in H^k(\Omega),\, g \in W^{k,\infty}(\Omega) &\implies fg \in H^k(\Omega), \qquad k \in \mathbb{N}_0; \\ h \in H^1(\partial\Omega),\, k \in W^{1,\infty}(\partial\Omega) &\implies hk \in H^1(\partial\Omega). \end{aligned} \tag{2.17}$$

For a function f on Ω we denote by $f|_{\partial\Omega}$ and $\partial_\nu f|_{\partial\Omega}$ the trace and the trace of the normal derivative (with normal vector pointing outwards), respectively. For $s > 3/2$ the trace mapping

$$H^s(\Omega) \ni f \mapsto \{f|_{\partial\Omega}, \partial_\nu f|_{\partial\Omega}\} \in H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega) \tag{2.18}$$

is the continuous extension of the trace mapping defined on C^∞-functions. Recall that for $s > 3/2$ the mapping (2.18) is surjective onto $H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega)$.

Besides the Sobolev spaces $H^s(\Omega)$ the spaces

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

equipped with the inner product $(\cdot, \cdot)_s + (\Delta \cdot, \Delta \cdot)$ and corresponding norm will be useful. Observe that for $s \geq 2$ the spaces $H^s_\Delta(\Omega)$ and $H^s(\Omega)$ coincide. We also note that $H^s_\Delta(\Omega), s \in (0, 2)$, can be viewed as an interpolation space between $H^2(\Omega)$ and $H^0_\Delta(\Omega)$, where the latter space coincides with the maximal domain of the Laplacian in $L^2(\Omega)$. By [59] the trace mapping can be extended to a continuous mapping

$$H^s_\Delta(\Omega) \ni f \mapsto \{f|_{\partial\Omega}, \partial_\nu f|_{\partial\Omega}\} \in H^{s-1/2}(\partial\Omega) \times H^{s-3/2}(\partial\Omega) \tag{2.19}$$

for all $s \in [0, 2)$, where each of the mappings

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

is surjective for $s \in [0, 2)$. We also recall that the first and second Green's identities hold for all $f, g \in H^{3/2}_\Delta(\Omega)$ and $h \in H^1(\Omega)$:

$$\left(-\Delta f, h\right)_{L^2(\Omega)} = \left(\nabla f, \nabla h\right)_{L^2(\Omega;\mathbb{C}^n)} - \left(\partial_\nu f|_{\partial\Omega}, h|_{\partial\Omega}\right)_{L^2(\partial\Omega)} \tag{2.20}$$

and

$$\begin{aligned} &\left(-\Delta f, g\right)_{L^2(\Omega)} - \left(f, -\Delta g\right)_{L^2(\Omega)} \\ &= \left(f|_{\partial\Omega}, \partial_\nu g|_{\partial\Omega}\right)_{L^2(\partial\Omega)} - \left(\partial_\nu f|_{\partial\Omega}, g|_{\partial\Omega}\right)_{L^2(\partial\Omega)}, \end{aligned} \tag{2.21}$$

cf. [42, 59] and, e.g. [11, Theorem 4.2].

2.4. Some Local Sobolev Spaces

Let Σ be a compact connected C^∞-hypersurface which separates the Euclidean space $\mathbb{R}^n$ into a bounded (interior) domain Ω_{i} and an unbounded (exterior) domain Ω_{e}. In particular, $\Sigma = \partial\Omega_{\mathrm{i}} = \partial\Omega_{\mathrm{e}}$. For $s \geq 0$ we use the short notation

$$
\begin{aligned}
H^s(\mathbb{R}^n\backslash\Sigma) &:= H^s(\Omega_{\mathrm{i}}) \oplus H^s(\Omega_{\mathrm{e}}), \\
H^s_\Delta(\mathbb{R}^n\backslash\Sigma) &:= H^s_\Delta(\Omega_{\mathrm{i}}) \oplus H^s_\Delta(\Omega_{\mathrm{e}}).
\end{aligned}
\tag{2.22}
$$

We denote by $H^s_\Sigma(\Omega_{\mathrm{i}})$ with $s \geq 0$ the subspace of $L^2(\Omega_{\mathrm{i}})$ which consists of functions that belong to H^s in a neighbourhood of $\Sigma = \partial\Omega_{\mathrm{i}}$, i.e.

$$
H^s_\Sigma(\Omega_{\mathrm{i}}) := \big\{ f \in L^2(\Omega_{\mathrm{i}}) \colon \exists \text{ domain } \Omega' \subset \Omega_{\mathrm{i}} \text{ such that }
$$
$$
\partial\Omega' \supset \Sigma \text{ and } f \restriction \Omega' \in H^s(\Omega') \big\}.
$$

The space $H^s_\Sigma(\Omega_{\mathrm{e}})$ is defined in the same way with Ω_{i} replaced by Ω_{e}. The local Sobolev spaces $H^s_\Sigma(\mathbb{R}^n)$ and $H^s_\Sigma(\mathbb{R}^n\backslash\Sigma)$ in the next definition consist of L^2-functions which are H^s in a neighbourhood of Σ or in both one-sided neighbourhoods of Σ, respectively.

Definition 2.9. Let $\Sigma, \Omega_{\mathrm{i}}, \Omega_{\mathrm{e}}$, and the spaces $H^s_\Sigma(\Omega_{\mathrm{i}})$ and $H^s_\Sigma(\Omega_{\mathrm{e}}), s \geq 0$, be as above. Then we define

$$
H^s_\Sigma(\mathbb{R}^n) := \big\{ f \in L^2(\mathbb{R}^n) \colon \exists \text{ domain } \Omega' \subset \mathbb{R}^n \text{ such that }
$$
$$
\Omega' \supset \Sigma \text{ and } f \restriction \Omega' \in H^s(\Omega') \big\},
$$
$$
H^s_\Sigma(\mathbb{R}^n\backslash\Sigma) := H^s_\Sigma(\Omega_{\mathrm{i}}) \oplus H^s_\Sigma(\Omega_{\mathrm{e}}).
$$

It follows from the above definition that $H^s_\Sigma(\mathbb{R}^n) \subsetneq H^s_\Sigma(\mathbb{R}^n\backslash\Sigma)$ holds for all $s > 0$.

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

$$
W^{k,\infty}_\Sigma(\Omega_{\mathrm{i}}) := \big\{ f \in L^\infty(\Omega_{\mathrm{i}}) \colon \exists \text{ domain } \Omega' \subset \Omega_{\mathrm{i}} \text{ such that }
$$
$$
\partial\Omega' \supset \Sigma \text{ and } f \restriction \Omega' \in W^{k,\infty}(\Omega') \big\}.
$$

The space $W^{k,\infty}_\Sigma(\Omega_{\mathrm{e}})$ is defined in the same way with Ω_{i} replaced by Ω_{e}. In analogy to Definition 2.9 we introduce the local Sobolev spaces $W^{k,\infty}_\Sigma(\mathbb{R}^n)$ and $W^{k,\infty}_\Sigma(\mathbb{R}^n\backslash\Sigma)$ of L^∞-functions which belong to $W^{k,\infty}$ in a neighbourhood or both one-sided neighbourhoods of Σ, respectively.

Definition 2.10. Let $\Sigma, \Omega_{\mathrm{i}}, \Omega_{\mathrm{e}}$, and the spaces $W^{k,\infty}_\Sigma(\Omega_{\mathrm{i}})$ and $W^{k,\infty}_\Sigma(\Omega_{\mathrm{e}}), k \in \mathbb{N}_0$, be as above. Then we define

$$
W^{k,\infty}_\Sigma(\mathbb{R}^n) := \big\{ f \in L^\infty(\mathbb{R}^n) \colon \exists \text{ domain } \Omega' \subset \mathbb{R}^n \text{ such that }
$$
$$
\Omega' \supset \Sigma \text{ and } f \restriction \Omega' \in W^{k,\infty}(\Omega') \big\},
$$
$$
W^{k,\infty}_\Sigma(\mathbb{R}^n\backslash\Sigma) := W^{k,\infty}_\Sigma(\Omega_{\mathrm{i}}) \times W^{k,\infty}_\Sigma(\Omega_{\mathrm{e}}).
$$

Finally, we recall a well-known result about the $\mathfrak{S}_{p,\infty}$ property of bounded operators mapping into the Sobolev space $H^{q_2}(\Sigma)$, where $q_2 > 0$ and $\Sigma = \partial\Omega_{\mathrm{i}} = \partial\Omega_{\mathrm{e}}$ is the $(n-1)$-dimensional compact connected C^∞-hypersurface from above, cf. [50] and [11, Lemma 4.6].

Lemma 2.11. *Let $\mathcal{K}$ be a Hilbert space, $B \in \mathcal{B}(\mathcal{K}, L^2(\Sigma))$ and let $q_2 > q_1 \geq 0$. If $\operatorname{ran} B \subset H^{q_2}(\Sigma)$, then B belongs to the class $\mathfrak{S}_{\frac{n-1}{q_2-q_1},\infty}(\mathcal{K}, H^{q_1}(\Sigma))$.*

3. Self-Adjoint Schrödinger Operators with δ and δ'-Interactions on Hypersurfaces

In this section we define the Schrödinger operators with δ and δ'-interactions on hypersurfaces with the help of quasi boundary triple techniques. These definitions coincide with the ones in the introduction and are compatible with those for one-dimensional δ-point interactions from [3,4] and the definition of δ-interactions on manifolds via quadratic forms; see, e.g. [18,35,39,41,58]. We also determine the semi-bounded closed quadratic form which corresponds to the Schrödinger operator with a δ'-interaction on a hypersurface, which answers a question from [30] posed by P. Exner. As a byproduct of the quasi boundary triple approach we obtain variants of Krein's formula and the Birman–Schwinger principle. This section contains the complete proofs of Theorem A and Theorem B from the introduction.

3.1. Notations and Preliminary Facts

Let Σ be a compact connected C^∞-hypersurface which separates the Euclidean space $\mathbb{R}^n, n \geq 2$, into a bounded (interior) domain Ω_i and an unbounded (exterior) domain Ω_e with the common boundary $\partial\Omega_i = \partial\Omega_e = \Sigma$. Let

$$\mathcal{L} = -\Delta + V, \tag{3.1}$$

where V is a real-valued potential from $L^\infty(\mathbb{R}^n)$. The restrictions of $\mathcal{L}$ to the interior and exterior domains will be denoted, respectively, by

$$\mathcal{L}_i = \mathcal{L} \restriction \Omega_i \quad \text{and} \quad \mathcal{L}_e = \mathcal{L} \restriction \Omega_e.$$

For a function $f \in L^2(\mathbb{R}^n)$ we write $f = f_i \oplus f_e$, where $f_i = f \restriction \Omega_i$ and $f_e = f \restriction \Omega_e$. Let us denote by $(\cdot,\cdot), (\cdot,\cdot)_i, (\cdot,\cdot)_e$ and $(\cdot,\cdot)_\Sigma$ the inner products in the Hilbert spaces $L^2(\mathbb{R}^n), L^2(\Omega_i), L^2(\Omega_e)$ and $L^2(\Sigma)$, respectively. When it is clear from the context, we denote the inner products in the Hilbert spaces $L^2(\mathbb{R}^n;\mathbb{C}^n), L^2(\Omega_i;\mathbb{C}^n)$, and $L^2(\Omega_e;\mathbb{C}^n)$ of vector-valued functions also by $(\cdot,\cdot), (\cdot,\cdot)_i$ and $(\cdot,\cdot)_e$, respectively.

The minimal operators associated with the differential expressions $\mathcal{L}_i$ and $\mathcal{L}_e$ are defined by

$$A_i f_i = \mathcal{L}_i f_i, \qquad \operatorname{dom} A_i = H_0^2(\Omega_i),$$
$$A_e f_e = \mathcal{L}_e f_e, \qquad \operatorname{dom} A_e = H_0^2(\Omega_e).$$

The operators A_i and A_e are densely defined closed symmetric operators with infinite deficiency indices in $L^2(\Omega_i)$ and $L^2(\Omega_e)$, respectively. Hence their direct sum

$$A_{i,e} = A_i \oplus A_e, \qquad \operatorname{dom} A_{i,e} = H_0^2(\Omega_i) \oplus H_0^2(\Omega_e), \tag{3.2}$$

is a densely defined closed symmetric operator with infinite deficiency indices in the space $L^2(\mathbb{R}^n) = L^2(\Omega_i) \oplus L^2(\Omega_e)$. Furthermore, we introduce the operators

$$T_i f_i = \mathcal{L}_i f_i, \qquad \operatorname{dom} T_i = H_\Delta^{3/2}(\Omega_i),$$

$$T_e f_e = \mathcal{L}_e f_e, \qquad \operatorname{dom} T_e = H_\Delta^{3/2}(\Omega_e),$$

and their direct sum

$$T_{i,e} = T_i \oplus T_e, \qquad \operatorname{dom} T_{i,e} = H_\Delta^{3/2}(\mathbb{R}^n \backslash \Sigma),$$

where the notation in (2.22) is used. It can be shown that $A_i^* = \overline{T}_i$, $A_e^* = \overline{T}_e$, and hence $A_{i,e}^* = \overline{T}_{i,e}$. Next we define the usual self-adjoint Dirichlet and Neumann realizations of the differential expressions $\mathcal{L}_i$ and $\mathcal{L}_e$ in $L^2(\Omega_i)$ and $L^2(\Omega_e)$, respectively:

$$A_{D,i} f_i = \mathcal{L}_i f_i, \qquad \operatorname{dom} A_{D,i} = \{f_i \in H^2(\Omega_i) \colon f_i|_\Sigma = 0\},$$

$$A_{D,e} f_e = \mathcal{L}_e f_e, \qquad \operatorname{dom} A_{D,e} = \{f_e \in H^2(\Omega_e) \colon f_e|_\Sigma = 0\},$$

$$A_{N,i} f_i = \mathcal{L}_i f_i, \qquad \operatorname{dom} A_{N,i} = \{f_i \in H^2(\Omega_i) \colon \partial_{\nu_i} f_i|_\Sigma = 0\},$$

$$A_{N,e} f_e = \mathcal{L}_e f_e, \qquad \operatorname{dom} A_{N,e} = \{f_e \in H^2(\Omega_e) \colon \partial_{\nu_e} f_e|_\Sigma = 0\},$$

and their direct sums

$$A_{D,i,e} = A_{D,i} \oplus A_{D,e},$$
$$\operatorname{dom} A_{D,i,e} = \{f \in H^2(\mathbb{R}^n \backslash \Sigma) : f_i|_\Sigma = f_e|_\Sigma = 0\}, \tag{3.3}$$

and

$$A_{N,i,e} = A_{N,i} \oplus A_{N,e},$$
$$\operatorname{dom} A_{N,i,e} = \{f \in H^2(\mathbb{R}^n \backslash \Sigma) : \partial_{\nu_i} f_i|_\Sigma = \partial_{\nu_e} f_e|_\Sigma = 0\}, \tag{3.4}$$

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

$$A_{\text{free}} f = \mathcal{L} f, \qquad \operatorname{dom} A_{\text{free}} = H^2(\mathbb{R}^n). \tag{3.5}$$

In the next proposition we define quasi boundary triples for A_i^* and A_e^*, and recall some properties of the associated γ-fields and Weyl functions; see [8, Proposition 4.6] and [11, Theorem 4.2]. For brevity we discuss the interior case $j = i$ and the exterior case $j = e$ simultaneously.

Proposition 3.1. *Let* $A_i, A_e, T_i, T_e, A_{D,i}, A_{D,e}, A_{N,i}$ *and* $A_{N,e}$ *be as above. Then the following statements hold for* $j = i$ *and* $j = e$.

(i) *The triple* $\Pi_j = \{L^2(\Sigma), \Gamma_{0,j}, \Gamma_{1,j}\}$, *where*

$$\Gamma_{0,j} f_j = \partial_{\nu_j} f_j|_\Sigma, \quad \Gamma_{1,j} f_j = f_j|_\Sigma, \quad f_j \in \operatorname{dom} T_j = H_\Delta^{3/2}(\Omega_j),$$

is a quasi boundary triple for A_j^*. *The restrictions of* T_j *to the kernels of the boundary mappings are the Neumann and Dirichlet operators:*

$$T_j \restriction \ker \Gamma_{0,j} = A_{N,j}, \quad T_j \restriction \ker \Gamma_{1,j} = A_{D,j};$$

the ranges of the boundary mappings are

$$\operatorname{ran} \Gamma_{0,j} = L^2(\Sigma) \quad and \quad \operatorname{ran} \Gamma_{1,j} = H^1(\Sigma).$$

(ii) *For $\lambda \in \rho(A_{N,j})$ and $\varphi \in L^2(\Sigma)$ the boundary value problem*

$$(\mathcal{L}_j - \lambda)f_j = 0, \qquad \partial_{\nu_j} f_j|_\Sigma = \varphi, \tag{3.6}$$

has the unique solution $\gamma_j(\lambda)\varphi \in H^{3/2}_\Delta(\Omega_j)$, where γ_j is the γ-field associated with Π_j. Moreover, $\gamma_j(\lambda)$ is bounded from $L^2(\Sigma)$ into $L^2(\Omega_j)$.

(iii) *For $\lambda \in \rho(A_{N,j})$ the Weyl function M_j associated with Π_j is given by*

$$M_j(\lambda)\varphi = f_j|_\Sigma, \qquad \varphi \in L^2(\Sigma),$$

where $f_j = \gamma_j(\lambda)\varphi$ is the solution of (3.6). The operators $M_j(\lambda)$ are bounded from $L^2(\Sigma)$ to $H^1(\Sigma)$ and compact in $L^2(\Sigma)$. If, in addition, $\lambda \in \rho(A_{D,j})$, then $M_j(\lambda)$ is a bijective map from $L^2(\Sigma)$ onto $H^1(\Sigma)$.

The operators $M_i(\lambda)$ and $M_e(\lambda)$ in Proposition 3.1 (iii) are the Neumann-to-Dirichlet maps associated with the differential expressions $\mathcal{L}_i - \lambda$ and $\mathcal{L}_e - \lambda$, respectively.

3.2. Schrödinger Operators with δ-Interactions on Hypersurfaces: Self-Adjointness, Krein's Formula and H^2-Regularity

In this section we make use of quasi boundary triples to define and study the Schrödinger operator $A_{\delta,\alpha}$ associated with the formal differential expression $\mathcal{L}_{\delta,\alpha} = -\Delta + V - \alpha\langle\delta_\Sigma, \cdot\rangle\delta_\Sigma$ in (1.1). It is convenient to use the symmetric extension

$$\widetilde{A} := A_{\text{free}} \cap A_{D,i,e} = \mathcal{L} \restriction \{f \in H^2(\mathbb{R}^n) : f_i|_\Sigma = f_e|_\Sigma = 0\} \tag{3.7}$$

of the orthogonal sum $A_{i,e}$ in (3.2) as the underlying symmetric operator for the quasi boundary triple. Furthermore,

$$\widetilde{T} := T_{i,e} \restriction \{f_i \oplus f_e \in H^{3/2}_\Delta(\mathbb{R}^n\backslash\Sigma) : f_i|_\Sigma = f_e|_\Sigma\} \tag{3.8}$$

acts as the operator on whose domain boundary mappings are defined in the next proposition. The method of intermediate extensions is inspired by the general considerations for ordinary boundary triples in [24, Section 4]. We remark that the quasi boundary triple and Weyl function below appear also implicitly in [5] and [66, Section 4] in a different context.

Proposition 3.2. *Let the operators $\widetilde{A}, \widetilde{T}, A_{D,i,e}, A_{N,i,e}$ and A_{free} be as in (3.7), (3.8), (3.3), (3.4) and (3.5), respectively, and let M_i and M_e be the Weyl functions from Proposition 3.1. Then the following statements hold.*

(i) *The triple $\widetilde{\Pi} = \{L^2(\Sigma), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$, where*

$$\widetilde{\Gamma}_0 f = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma, \quad \widetilde{\Gamma}_1 f = f|_\Sigma, \qquad f = f_i \oplus f_e \in \text{dom}\,\widetilde{T},$$

is a quasi boundary triple for $\widetilde{A}^*$. The restrictions of $\widetilde{T}$ to the kernels of the boundary mappings are

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

and the ranges of the boundary mappings are

$$\text{ran}\,\widetilde{\Gamma}_0 = L^2(\Sigma) \quad and \quad \text{ran}\,\widetilde{\Gamma}_1 = H^1(\Sigma). \tag{3.9}$$

(ii) *For $\lambda \in \rho(A_{\mathrm{free}})$ and $\varphi \in L^2(\Sigma)$ the transmission problem*

$$(\mathcal{L} - \lambda)f = 0, \qquad f_{\mathrm{e}}|_{\Sigma} = f_{\mathrm{i}}|_{\Sigma}, \quad \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_{\Sigma} + \partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_{\Sigma} = \varphi, \qquad (3.10)$$

has the unique solution $\widetilde{\gamma}(\lambda)\varphi \in H_{\Delta}^{3/2}(\mathbb{R}^n \backslash \Sigma)$, where $\widetilde{\gamma}$ is the γ-field associated with $\widetilde{\Pi}$. Moreover, $\widetilde{\gamma}(\lambda)$ is bounded from $L^2(\Sigma)$ to $L^2(\mathbb{R}^n)$.

(iii) *For $\lambda \in \rho(A_{\mathrm{free}})$ the values $\widetilde{M}(\lambda)$ of the Weyl function associated with $\widetilde{\Pi}$ are bounded operators from $L^2(\Sigma)$ to $H^1(\Sigma)$ and compact operators in $L^2(\Sigma)$. If, in addition, $\lambda \in \rho(A_{\mathrm{D,i,e}})$, then $\widetilde{M}(\lambda)$ is a bijective map from $L^2(\Sigma)$ onto $H^1(\Sigma)$. Moreover, the identity*

$$\widetilde{M}(\lambda) = \left(M_{\mathrm{i}}(\lambda)^{-1} + M_{\mathrm{e}}(\lambda)^{-1} \right)^{-1} \qquad (3.11)$$

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) First note that the boundary mappings $\widetilde{\Gamma}_0, \widetilde{\Gamma}_1$ are well defined because of the properties of the trace mappings (2.19). We show that the triple $\widetilde{\Pi}$ satisfies the conditions (a), (b) and (c) in Proposition 2.5. For condition (a), let $\varphi \in H^{1/2}(\Sigma)$ and $\psi \in H^{3/2}(\Sigma)$ be arbitrary. By (2.18) 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 $H^2(\mathbb{R}^n \backslash \Sigma) \subset H_{\Delta}^{3/2}(\mathbb{R}^n \backslash \Sigma)$, we have $f := f_{\mathrm{i}} \oplus f_{\mathrm{e}} \in \mathrm{dom}\,\widetilde{T}$ and $\widetilde{\Gamma}_0 f = \varphi, \widetilde{\Gamma}_1 f = \psi$. Hence

$$H^{1/2}(\Sigma) \times H^{3/2}(\Sigma) \subset \mathrm{ran}\begin{pmatrix} \widetilde{\Gamma}_0 \\ \widetilde{\Gamma}_1 \end{pmatrix},$$

which implies that the first item in (a) of Proposition 2.5 is satisfied; the second item is clear. Next let $f = f_{\mathrm{i}} \oplus f_{\mathrm{e}}$ and $g = g_{\mathrm{i}} \oplus g_{\mathrm{e}}$ be two arbitrary functions in $\mathrm{dom}\,\widetilde{T}$. From Green's identity (2.21) we obtain the following two equalities:

$$(T_{\mathrm{i}} f_{\mathrm{i}}, g_{\mathrm{i}})_{\mathrm{i}} - (f_{\mathrm{i}}, T_{\mathrm{i}} g_{\mathrm{i}})_{\mathrm{i}} = \left(f_{\mathrm{i}}|_{\Sigma}, \partial_{\nu_{\mathrm{i}}} g_{\mathrm{i}}|_{\Sigma} \right)_{\Sigma} - \left(\partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_{\Sigma}, g_{\mathrm{i}}|_{\Sigma} \right)_{\Sigma},$$
$$(T_{\mathrm{e}} f_{\mathrm{e}}, g_{\mathrm{e}})_{\mathrm{e}} - (f_{\mathrm{e}}, T_{\mathrm{e}} g_{\mathrm{e}})_{\mathrm{e}} = \left(f_{\mathrm{e}}|_{\Sigma}, \partial_{\nu_{\mathrm{e}}} g_{\mathrm{e}}|_{\Sigma} \right)_{\Sigma} - \left(\partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_{\Sigma}, g_{\mathrm{e}}|_{\Sigma} \right)_{\Sigma}.$$

Since the functions f and g in $\mathrm{dom}\,\widetilde{T}$ satisfy the boundary conditions

$$f_{\mathrm{i}}|_{\Sigma} = f_{\mathrm{e}}|_{\Sigma} = f|_{\Sigma} \quad \text{and} \quad g_{\mathrm{i}}|_{\Sigma} = g_{\mathrm{e}}|_{\Sigma} = g|_{\Sigma},$$

we have

$$\left(\widetilde{T} f, g \right) - \left(f, \widetilde{T} g \right) = (T_{\mathrm{i}} f_{\mathrm{i}}, g_{\mathrm{i}})_{\mathrm{i}} - (f_{\mathrm{i}}, T_{\mathrm{i}} g_{\mathrm{i}})_{\mathrm{i}} + (T_{\mathrm{e}} f_{\mathrm{e}}, g_{\mathrm{e}})_{\mathrm{e}} - (f_{\mathrm{e}}, T_{\mathrm{e}} g_{\mathrm{e}})_{\mathrm{e}}$$
$$= \left(f|_{\Sigma}, \partial_{\nu_{\mathrm{i}}} g_{\mathrm{i}}|_{\Sigma} + \partial_{\nu_{\mathrm{e}}} g_{\mathrm{e}}|_{\Sigma} \right)_{\Sigma} - \left(\partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_{\Sigma} + \partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_{\Sigma}, g|_{\Sigma} \right)_{\Sigma},$$

which shows that condition (b) of Proposition 2.5 is fulfilled. Since the restriction $\widetilde{T} \upharpoonright \ker \widetilde{\Gamma}_0$ contains the self-adjoint operator A_{free}, also condition (c) is satisfied. Hence we can apply Proposition 2.5, which implies that

$$\widetilde{T} \upharpoonright (\ker \widetilde{\Gamma}_0 \cap \ker \widetilde{\Gamma}_1)$$

is a densely defined closed symmetric operator in $L^2(\mathbb{R}^n)$, that the triple $\widetilde{\Pi} = \{L^2(\Sigma), \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is a quasi boundary triple for its adjoint and that

$$A_{\text{free}} = \widetilde{T} \restriction \ker \widetilde{\Gamma}_0.$$

Note that the operator $\widetilde{T} \restriction \ker \widetilde{\Gamma}_1$ is symmetric by Green's identity and contains the self-adjoint operator $A_{\text{D,i,e}}$. Therefore these operators also coincide. Hence we get

$$\widetilde{T} \restriction (\ker \widetilde{\Gamma}_0 \cap \ker \widetilde{\Gamma}_1) = \left(\widetilde{T} \restriction \ker \widetilde{\Gamma}_0\right) \cap \left(\widetilde{T} \restriction \ker \widetilde{\Gamma}_1\right) = A_{\text{free}} \cap A_{\text{D,i,e}} = \widetilde{A}.$$

Since, for $j = \text{i}$ and $j = \text{e}$, the mapping $f_j \mapsto f_j|_\Sigma$ is surjective from $H_\Delta^{3/2}(\Omega_j)$ onto $H^1(\Sigma)$ and the mapping $f_j \mapsto \partial_{\nu_j} f_j|_\Sigma$ is surjective from $H_\Delta^{3/2}(\Omega_j)$ onto $L^2(\Sigma)$, it follows easily that $\operatorname{ran} \widetilde{\Gamma}_1 = H^1(\Sigma)$ and that $\operatorname{ran} \widetilde{\Gamma}_0 \subset L^2(\Sigma)$. 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 $\overline{\Omega_i}$. Let SL be the single-layer potential associated with the hypersurface Σ and the differential expression $-\Delta + 1$; see, e.g. [62, Chapter 6] for the definition and properties of single-layer potentials. By [62, Theorem 6.11, Theorem 6.12 (i)], for an arbitrary $\varphi \in L^2(\Sigma)$, the function $f := \chi \text{SL} \varphi$ belongs to $\operatorname{dom} \widetilde{T}$ and satisfies the condition

$$\partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma = \varphi,$$

hence $\widetilde{\Gamma}_0 f = \varphi$, and thus $\operatorname{ran} \widetilde{\Gamma}_0 = L^2(\Sigma)$.

(ii) For $\lambda \in \rho(A_{\text{free}})$ the γ-field $\widetilde{\gamma}(\lambda)$ associated with the quasi boundary triple $\widetilde{\Pi}$ maps $\operatorname{ran} \widetilde{\Gamma}_0 = L^2(\Sigma)$ onto $\ker(\widetilde{T} - \lambda)$ by Definition 2.6 and Proposition 2.7 (i). Hence $f = f_i \oplus f_e := \widetilde{\gamma}(\lambda)\varphi$ satisfies

$$(\mathcal{L} - \lambda)f = 0, \quad f \in H^{3/2}(\mathbb{R}^n \backslash \Sigma) \quad \text{and} \quad f_i|_\Sigma = f_e|_\Sigma.$$

Furthermore,

$$\varphi = \widetilde{\Gamma}_0 \widetilde{\gamma}(\lambda)\varphi = \widetilde{\Gamma}_0 f = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma$$

and hence $f = \widetilde{\gamma}(\lambda)\varphi$ is the unique solution of the problem (3.10).

(iii) Definition 2.6, Proposition 2.7 (iv) and (v) and (3.9) imply that $\widetilde{M}(\lambda)$ is a bounded operator from $L^2(\Sigma)$ into $H^1(\Sigma)$ for $\lambda \in \rho(A_{\text{free}})$ and that it is bijective for $\lambda \in \rho(A_{\text{free}}) \cap \rho(A_{\text{D,i,e}})$. The compactness of $\widetilde{M}(\lambda)$ in $L^2(\Sigma)$ is a consequence of the compactness of the embedding of $H^1(\Sigma)$ into $L^2(\Sigma)$; see, e.g. [71, Theorem 7.10].

In order to prove the identity (3.11), let $\lambda \in \rho(A_{\text{free}}) \cap \rho(A_{\text{D,i,e}}) \cap \rho(A_{\text{N,i,e}})$. For such λ the operator $\widetilde{M}(\lambda)$ is invertible, and the same holds true for $M_i(\lambda)$ and $M_e(\lambda)$; cf. Proposition 3.1. If $\widetilde{M}(\lambda)\varphi = \psi$ for some $\varphi \in L^2(\Sigma)$ and $\psi \in H^1(\Sigma)$, then there exists an $f = f_i \oplus f_e \in \ker(\widetilde{T} - \lambda)$ such that

$$\widetilde{\Gamma}_0 f = \varphi \qquad \text{and} \qquad \widetilde{\Gamma}_1 f = \psi.$$

As $f_i \in \ker(T_i - \lambda)$ and $f_e \in \ker(T_e - \lambda)$, we have

$$\Gamma_{0,i} f_i = M_i(\lambda)^{-1} \Gamma_{1,i} f_i = M_i(\lambda)^{-1} \psi,$$
$$\Gamma_{0,e} f_e = M_e(\lambda)^{-1} \Gamma_{1,e} f_e = M_e(\lambda)^{-1} \psi,$$

and hence

$$\widetilde{M}(\lambda)^{-1} \psi = \varphi = \partial_{\nu_i} f_i|_\Sigma + \partial_{\nu_e} f_e|_\Sigma = \Gamma_{0,i} f_i + \Gamma_{0,e} f_e$$
$$= M_i(\lambda)^{-1} \psi + M_e(\lambda)^{-1} \psi.$$

Since this is true for arbitrary $\psi \in H^1(\Sigma)$, relation (3.11) follows. $\qquad\square$

Remark 3.3. Assume for simplicity that the potential V in the differential expression $\mathcal{L}$ in (3.1) is identically equal to zero. In this case the γ-field $\widetilde{\gamma}$ and the Weyl function $\widetilde{M}$ in Proposition 3.2 are, roughly speaking, extensions of the acoustic single-layer potential for the Helmholtz equation. In fact, if $G_\lambda, \lambda \in \mathbb{C}\backslash\mathbb{R}$, is the integral kernel of the resolvent of A_{free}, then for all $\varphi \in C^\infty(\Sigma)$ we have

$$(\widetilde{\gamma}(\lambda)\varphi)(x) = \int_\Sigma G_\lambda(x,y)\varphi(y)d\sigma_y, \quad x \in \mathbb{R}^n\backslash\Sigma,$$

and

$$(\widetilde{M}(\lambda)\varphi)(x) = \int_\Sigma G_\lambda(x,y)\varphi(y)d\sigma_y, \quad x \in \Sigma,$$

where σ_y is the natural Lebesgue measure on Σ. For more details we refer the reader to [62, Chapter 6]; see also [21,22].

We repeat the definition of a Schrödinger operator with δ-potential from the introduction and relate it to the quasi boundary triple $\widetilde{\Pi}$.

Definition 3.4. 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:

$$A_{\delta,\alpha} := \widetilde{T} \restriction \ker(\alpha\widetilde{\Gamma}_1 - \widetilde{\Gamma}_0),$$

which is equivalent to

$$A_{\delta,\alpha} f := -\Delta f + Vf,$$
$$\operatorname{dom} A_{\delta,\alpha} := \left\{ f \in H_\Delta^{3/2}(\mathbb{R}^n\backslash\Sigma) : \begin{array}{l} f_i|_\Sigma = f_e|_\Sigma = f|_\Sigma \\ \alpha f|_\Sigma = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma \end{array} \right\}. \tag{3.12}$$

The definition of $A_{\delta,\alpha}$ is compatible with the definition of a point δ-interaction in the one-dimensional case [3, Section I.3], [4] and the definitions of the operators with δ-potentials on hypersurfaces given in [6,67] and in [18]; see also Proposition 3.7. Note also that the domain of $A_{\delta,\alpha}$ is contained in $H^1(\mathbb{R}^n)$; cf. Proposition 3.7. For the relation between the operator $A_{\delta,\alpha}$ and the other operators studied in this section see Fig. 1.

The following theorem contains a proof of self-adjointness of the operator $A_{\delta,\alpha}$ and provides a factorization for the resolvent difference of $A_{\delta,\alpha}$ and A_{free}
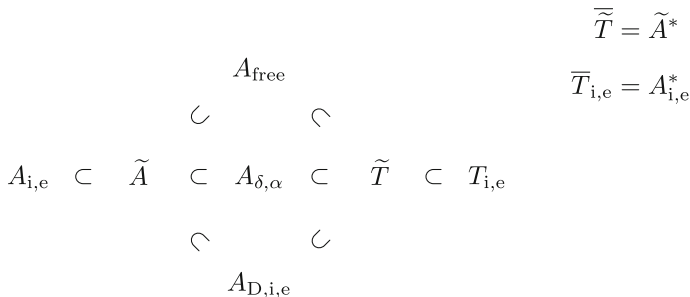
$$\overline{\widetilde{T}} = \widetilde{A}^*$$

$$\overline{T}_{\mathrm{i,e}} = A^*_{\mathrm{i,e}}$$

$$A_{\mathrm{free}}$$

$$A_{\mathrm{i,e}} \quad \subset \quad \widetilde{A} \quad \subset \quad A_{\delta,\alpha} \quad \subset \quad \widetilde{T} \quad \subset \quad T_{\mathrm{i,e}}$$

$$A_{\mathrm{D,i,e}}$$

FIGURE 1. This figure shows how the operator $A_{\delta,\alpha}$ is related to the other operators studied in this section. The operators $A_{\mathrm{free}}, A_{\delta,\alpha}$ and $A_{\mathrm{D,i,e}}$ are self-adjoint

via Krein's formula; cf. [18, Lemma 2.3 (iii)]. Item (iii) in Theorem 3.5 can be viewed as a variant of the Birman–Schwinger principle; it coincides with the one in [18]. The first item of Theorem 3.5 is part of Theorem A in the introduction.

Theorem 3.5. *Let $A_{\delta,\alpha}$ be as above and let A_{free} be the self-adjoint operator defined in (3.5). Let $\widetilde{\gamma}$ and $\widetilde{M}$ be the γ-field and the Weyl function associated with the quasi boundary triple $\widetilde{\Pi}$ from Proposition 3.2. 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 $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\mathrm{free}})$ the following Krein formula holds:*

$$(A_{\delta,\alpha} - \lambda)^{-1} - (A_{\mathrm{free}} - \lambda)^{-1} = \widetilde{\gamma}(\lambda)\left(I - \alpha\widetilde{M}(\lambda)\right)^{-1}\alpha\,\widetilde{\gamma}(\overline{\lambda})^*,$$

where $(I - \alpha\widetilde{M}(\lambda))^{-1} \in \mathcal{B}(L^2(\Sigma))$.
(iii) *For all $\lambda \in \mathbb{R}\backslash\sigma(A_{\mathrm{free}})$ we have*

$$\lambda \in \sigma_p(A_{\delta,\alpha}) \quad \Longleftrightarrow \quad 0 \in \sigma_p\big(I - \alpha\widetilde{M}(\lambda)\big)$$

and $\dim\ker(A_{\delta,\alpha} - \lambda) = \dim\ker(I - \alpha\widetilde{M}(\lambda))$.

Proof. Under our assumptions on the function α the operator of multiplication with α is bounded and self-adjoint in the Hilbert space $L^2(\Sigma)$. The values of the Weyl function $\widetilde{M}$ are compact operators in $L^2(\Sigma)$; see Proposition 3.2 (iii). Now the assertions (i)–(iii) follow from Theorem 2.8. $\qquad\square$

The next theorem gives assumptions on α, which ensure that the domain of the self-adjoint operator $A_{\delta,\alpha}$ has H^2-regularity in $\mathbb{R}^n\backslash\Sigma$. This theorem is the first part of Theorem B in the introduction. Recall that $W^{1,\infty}(\Sigma)$ is the Sobolev space of order one of L^∞ functions on Σ; cf. Sect. 2.3.

Theorem 3.6. *Let $A_{\delta,\alpha}$ be the self-adjoint Schrödinger operator in Definition 3.4 and assume, in addition, that the function $\alpha\colon \Sigma \to \mathbb{R}$ belongs to $W^{1,\infty}(\Sigma)$. Then $\mathrm{dom}\,A_{\delta,\alpha}$ is contained in $H^2(\mathbb{R}^n\backslash\Sigma)$.*

Proof. For any function $f \in \operatorname{dom} A_{\delta,\alpha}$ we have $f \in \operatorname{dom} \widetilde{T} \subset H_{\Delta}^{3/2}(\mathbb{R}^n \backslash \Sigma)$. Then by Proposition 3.2 (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 (2.17) imply that

$$\widetilde{\Gamma}_0 f = \alpha \widetilde{\Gamma}_1 f \in H^1(\Sigma). \tag{3.13}$$

Let us fix $\lambda \in \mathbb{C} \backslash \mathbb{R}$. By the standard decomposition

$$\operatorname{dom} \widetilde{T} = \operatorname{dom} A_{\text{free}} \dotplus \ker(\widetilde{T} - \lambda) \tag{3.14}$$

the function $f \in \operatorname{dom} A_{\delta,\alpha}$ can be represented in the form $f = f_{\text{free}} + f_\lambda$, where $f_{\text{free}} \in \operatorname{dom} A_{\text{free}}$ and $f_\lambda \in \ker(\widetilde{T} - \lambda)$. It is clear that

$$f_{\text{free}} \in H^2(\mathbb{R}^n) \subset H^2(\mathbb{R}^n \backslash \Sigma).$$

Relation (3.13) and $A_{\text{free}} = \widetilde{T} \upharpoonright \ker \widetilde{\Gamma}_0$ yield

$$\widetilde{\Gamma}_0 f_\lambda = \widetilde{\Gamma}_0 f \in H^1(\Sigma) \subset H^{1/2}(\Sigma). \tag{3.15}$$

The properties of the trace map in (2.18) show that $\widetilde{\Gamma}_0$ maps the space $\operatorname{dom} \widetilde{T} \cap H^2(\mathbb{R}^n \backslash \Sigma)$ onto $H^{1/2}(\Sigma)$, and hence (3.14) implies that $\widetilde{\Gamma}_0$ maps

$$\ker(\widetilde{T} - \lambda) \cap H^2(\mathbb{R}^n \backslash \Sigma)$$

bijectively onto $H^{1/2}(\Sigma)$. This observation and (3.15) show $f_\lambda \in H^2(\mathbb{R}^n \backslash \Sigma)$, and therefore $f = f_{\text{free}} + f_\lambda \in H^2(\mathbb{R}^n \backslash \Sigma)$. $\qquad\square$

It follows from the proof that for Theorem 3.6 to hold it is sufficient that the multiplication by α maps $H^1(\Sigma)$-functions into $H^{1/2}(\Sigma)$.

A common method to define self-adjoint Schrödinger operators with δ-interactions on hypersurfaces makes use of semi-bounded closed sesquilinear forms. For this consider the sesquilinear form

$$\mathfrak{a}_{\delta,\alpha}[f,g] = (\nabla f, \nabla g) + (Vf, g) - (\alpha f|_\Sigma, g|_\Sigma)_\Sigma, \qquad f, g \in H^1(\mathbb{R}^n). \tag{3.16}$$

As it is shown in [18], for a real-valued $\alpha \in L^\infty(\Sigma)$ and a real-valued $V \in L^\infty(\mathbb{R}^n)$, the form $\mathfrak{a}_{\delta,\alpha}$ is semi-bounded, closed and symmetric. The first representation theorem—see [56, Theorem VI.2.1] or [64, Theorem VIII.15]—yields that a unique self-adjoint operator $\mathcal{A}_{\delta,\alpha}$ in $L^2(\mathbb{R}^n)$ corresponds to the form $\mathfrak{a}_{\delta,\alpha}$ in the sense that

$$(\mathcal{A}_{\delta,\alpha} f, g) = \mathfrak{a}_{\delta,\alpha}[f,g] \qquad \text{for all } f \in \operatorname{dom} \mathcal{A}_{\delta,\alpha} \text{ and } g \in \operatorname{dom} \mathfrak{a}_{\delta,\alpha} = H^1(\mathbb{R}^n).$$

In the next proposition we show that our approach leads to the same operator.

Proposition 3.7. *The self-adjoint Schrödinger operator $A_{\delta,\alpha}$ in Definition 3.4 and the self-adjoint operator $\mathcal{A}_{\delta,\alpha}$ corresponding to the sesquilinear form in (3.16) coincide.*

Proof. First we show the inclusion $\operatorname{dom} A_{\delta,\alpha} \subset \operatorname{dom} \mathfrak{a}_{\delta,\alpha}$. For this let $f = f_i \oplus f_e \in \operatorname{dom} A_{\delta,\alpha}$. According to (3.12) we have, in particular,

$$f_i \in H^{3/2}(\Omega_i) \subset H^1(\Omega_i), \quad f_e \in H^{3/2}(\Omega_e) \subset H^1(\Omega_e), \quad \text{and} \quad f_i|_\Sigma = f_e|_\Sigma.$$

Making use of [2, Theorems 5.24 and 5.29] a standard extension argument implies that $f \in H^1(\mathbb{R}^n)$ and hence $\operatorname{dom} A_{\delta,\alpha} \subset \operatorname{dom} \mathfrak{a}_{\delta,\alpha}$.

Next let $f = f_i \oplus f_e \in \operatorname{dom} A_{\delta,\alpha}$ and $g = g_i \oplus g_e \in \operatorname{dom} \mathfrak{a}_{\delta,\alpha}$. Then $\mathfrak{a}_{\delta,\alpha}[f,g]$ is well defined. By the first Green's identity (2.20) we have

$$(\nabla f_i, \nabla g_i)_i - (\partial_{\nu_i} f_i|_\Sigma, g_i|_\Sigma)_\Sigma = (-\Delta f_i, g_i)_i,$$
$$(\nabla f_e, \nabla g_e)_e - (\partial_{\nu_e} f_e|_\Sigma, g_e|_\Sigma)_\Sigma = (-\Delta f_e, g_e)_e.$$

Using this and the relation $\alpha f|_\Sigma = \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma$ we obtain

$$\begin{aligned}
\mathfrak{a}_{\delta,\alpha}[f,g] &= (\nabla f, \nabla g) + (Vf, g) - \big(\alpha f|_\Sigma, g|_\Sigma\big)_\Sigma \\
&= (\nabla f_i, \nabla g_i)_i + (\nabla f_e, \nabla g_e)_e + (Vf, g) - \big(\partial_{\nu_i} f_i|_\Sigma, g_i|_\Sigma\big)_\Sigma - \big(\partial_{\nu_e} f_e|_\Sigma, g_e|_\Sigma\big)_\Sigma \\
&= (-\Delta f_i, g_i)_i + (-\Delta f_e, g_e)_e + (Vf, g) = \big((-\Delta + V)f, g\big).
\end{aligned}$$

Now the first representation theorem (see [56, Theorem VI.2.1]) implies that $f \in \operatorname{dom} \mathcal{A}_{\delta,\alpha}$ and $\mathcal{A}_{\delta,\alpha} f = -\Delta f + V f$; thus $A_{\delta,\alpha} \subset \mathcal{A}_{\delta,\alpha}$. Since both operators $A_{\delta,\alpha}$ and $\mathcal{A}_{\delta,\alpha}$ are self-adjoint, we conclude that $A_{\delta,\alpha} = \mathcal{A}_{\delta,\alpha}$. $\square$

3.3. Schrödinger Operators with δ'-Interactions on Hypersurfaces: Self-Adjointness, Krein's Formula and H^2-Regularity

In this section we make use of quasi boundary triples to define and study the Schrödinger operator $A_{\delta',\beta}$ associated with the formal differential expression $\mathcal{L}_{\delta,\alpha} = -\Delta + V - \beta\langle \delta'_\Sigma, \cdot \rangle \delta'_\Sigma$ in (1.1). The methodology and presentation is very much the same as in the previous section. We mention that to the best of our knowledge a systematic treatment of δ'-potentials on hypersurfaces is not contained elsewhere; see the list of open problems in [30].

In analogy to (3.7) and (3.8) we define the symmetric extension

$$\widehat{A} := A_{\text{free}} \cap A_{\text{N,i,e}} = \mathcal{L} \upharpoonright \{f \in H^2(\mathbb{R}^n) : \partial_{\nu_i} f_i|_\Sigma = \partial_{\nu_e} f_e|_\Sigma = 0\} \quad (3.17)$$

of the orthogonal sum $A_{i,e}$, defined in (3.2), which will serve as the underlying symmetric operator for the quasi boundary triple in the next proposition, and the operator

$$\widehat{T} := T_{i,e} \upharpoonright \{f_i \oplus f_e \in H^{3/2}_\Delta(\mathbb{R}^n \backslash \Sigma) : \partial_{\nu_e} f_e|_\Sigma + \partial_{\nu_i} f_i|_\Sigma = 0\}. \quad (3.18)$$

We remark that the quasi boundary triple and Weyl function below appear also implicitly in [66, Section 4] in a different context.

Proposition 3.8. *Let the operators $\widehat{A}, \widehat{T}, A_{\text{D,i,e}}, A_{\text{N,i,e}}$ and A_{free} be as in (3.17), (3.18), (3.3), (3.4) and (3.5), respectively, and let M_i and M_e be the Weyl functions from Proposition 3.1. Then the following statements hold.*

(i) *The triple $\widehat{\Pi} = \{L^2(\Sigma), \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$, where*

$$\widehat{\Gamma}_0 f = \partial_{\nu_e} f_e|_\Sigma, \quad \widehat{\Gamma}_1 f = f_e|_\Sigma - f_i|_\Sigma, \qquad f = f_i \oplus f_e \in \operatorname{dom} \widehat{T},$$

is a quasi boundary triple for $\widehat{A}^*$. The restrictions of $\widehat{T}$ to the kernels of the boundary mappings are

$$\widehat{T} \restriction \ker \widehat{\Gamma}_0 = A_{\mathrm{N,i,e}} \quad and \quad \widehat{T} \restriction \ker \widehat{\Gamma}_1 = A_{\mathrm{free}},$$

and the ranges of the boundary mappings are

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

(ii) *For $\lambda \in \rho(A_{\mathrm{N,i,e}})$ and $\varphi \in L^2(\Sigma)$ the problem*

$$(\mathcal{L} - \lambda)f = 0, \qquad \partial_{\nu_e} f_e|_\Sigma = -\partial_{\nu_i} f_i|_\Sigma = \varphi,$$

has the unique solution $\widehat{\gamma}(\lambda)\varphi \in H_\Delta^{3/2}(\mathbb{R}^n \backslash \Sigma)$, where $\widehat{\gamma}$ is the γ-field associated with $\widehat{\Pi}$. Moreover, $\widehat{\gamma}(\lambda)$ is bounded from $L^2(\Sigma)$ to $L^2(\mathbb{R}^n)$.

(iii) *For $\lambda \in \rho(A_{\mathrm{N,i,e}})$ the values $\widehat{M}(\lambda)$ of the Weyl function associated with $\widehat{\Pi}$ are bounded operators from $L^2(\Sigma)$ to $H^1(\Sigma)$ and compact operators in $L^2(\Sigma)$. If, in addition, $\lambda \in \rho(A_{\mathrm{free}})$, then $\widehat{M}(\lambda)$ is a bijective map from $L^2(\Sigma)$ onto $H^1(\Sigma)$. Moreover, the identity*

$$\widehat{M}(\lambda) = M_{\mathrm{i}}(\lambda) + M_{\mathrm{e}}(\lambda) \tag{3.19}$$

holds for all $\lambda \in \rho(A_{\mathrm{N,i,e}})$.

Proof. (i) One can see that $\widehat{\Pi}$ is a quasi boundary triple for $\widehat{A}^*$ in a similar way as in the proof of Proposition 3.2 (i). Basically, the same argumentation as before yields that $\widehat{T} \restriction \ker \widehat{\Gamma}_0 = A_{\mathrm{N,i,e}}, \widehat{T} \restriction \ker \widehat{\Gamma}_1 = A_{\mathrm{free}}$ and also 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 3.2, i.e. such that $\chi \equiv 1$ on an open neighbourhood of $\overline{\Omega_i}$. Let DL be the double-layer potential associated with the hypersurface Σ and the differential expression $-\Delta + 1$; see, e.g. [62, Section 6] for the discussion of double-layer potentials. By [62, 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

$$f_e|_\Sigma - f_i|_\Sigma = \varphi,$$

hence $\widehat{\Gamma}_1 f = \varphi$, and thus $\operatorname{ran} \widehat{\Gamma}_1 = H^1(\Sigma)$.

(ii)–(iii) The properties of the γ-field $\widehat{\gamma}$ and the Weyl function $\widehat{M}$ follow from Proposition 2.7 in the same way as in the proof of Proposition 3.2 (ii)–(iii). We only verify the identity (3.19). 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; cf. Proposition 3.1. If $\widehat{M}(\lambda)\varphi = \psi$ for some $\varphi \in L^2(\Sigma)$ and $\psi \in H^1(\Sigma)$, then there exists $f = f_i \oplus f_e \in \ker(\widehat{T} - \lambda)$ such that

$$\widehat{\Gamma}_0 f = \varphi \quad and \quad \widehat{\Gamma}_1 f = \psi.$$

As $f_i \in \ker(T_i - \lambda)$ and $f_e \in \ker(T_e - \lambda)$, we have

$$\Gamma_{1,i} f_i = M_i(\lambda)\Gamma_{0,i} f_i = -M_i(\lambda)\varphi,$$
$$\Gamma_{1,e} f_e = M_e(\lambda)\Gamma_{0,e} f_e = M_e(\lambda)\varphi,$$

and hence

$$\widehat{M}(\lambda)\varphi = f_e|_\Sigma - f_i|_\Sigma = M_e(\lambda)\varphi + M_i(\lambda)\varphi.$$

Since this is true for arbitrary $\varphi \in L^2(\Sigma)$, relation (3.19) follows. $\qquad\square$

Remark 3.9. Assume for simplicity that the potential V in the differential expression $\mathcal{L}$ in (3.1) is identically equal to zero. Note that the problem in Proposition 3.8 (ii) is decoupled into an interior and an exterior problem. Let, as in Remark 3.3, G_λ be the integral kernel of the resolvent of A_{free}. Then, for all $\psi \in C^\infty(\Sigma)$,

$$\big(\widehat{\gamma}(\lambda)\psi\big)(x) = \int_\Sigma \big[\partial_{\nu_i(y)}G_\lambda(x,y)\big]\big(\widehat{M}(\lambda)\psi\big)(y)d\sigma_y, \quad x \in \mathbb{R}^n\backslash\Sigma,$$

and

$$\big(\widehat{M}(\lambda)^{-1}\psi\big)(x) = -\partial_{\nu_i(x)}\int_\Sigma \big[\partial_{\nu_i(y)}G_\lambda(x,y)\big]\psi(y)d\sigma_y, \quad x \in \Sigma,$$

where $\partial_{\nu_i(x)}$ and $\partial_{\nu_i(y)}$ are the normal derivatives with respect to the first and second arguments with normals pointing outwards of Ω_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 $-\widehat{M}(\lambda)^{-1}$ coincides with the hypersingular operator; see, e.g. [62, Chapter 6] and [21, 22]. The representation of $\widehat{M}(\lambda)^{-1}$, given above, appears also in [66] in a slightly different context.

We repeat the definition of the Schrödinger operator with δ'-potential from the introduction and relate it to the quasi boundary triple $\widehat{\Pi}$.

Definition 3.10. 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

$$A_{\delta',\beta}f := -\Delta f + Vf,$$

$$\text{dom } A_{\delta',\beta} := \left\{ f \in H_\Delta^{3/2}(\mathbb{R}^n\backslash\Sigma) : \begin{array}{c} \partial_{\nu_e}f_e|_\Sigma = -\partial_{\nu_i}f_i|_\Sigma \\ \beta\partial_{\nu_e}f_e|_\Sigma = f_e|_\Sigma - f_i|_\Sigma \end{array} \right\}. \qquad (3.20)$$

The definition of $A_{\delta',\beta}$ is compatible with the definition of a point δ'-interaction in the one-dimensional case [3, Section I.4], [4] and the definition of the operator with δ'-potentials on spheres given in [6, 68]. Note that, in contrast to the domain of $A_{\delta,\alpha}$, the domain of $A_{\delta',\beta}$ is not contained in $H^1(\mathbb{R}^n)$. For the relation between the operator $A_{\delta',\beta}$ and the other operators studied in this section see Fig. 2.

The next theorem is the counterpart of Theorem 3.5 and can be proved in the same way. Theorem 3.11 shows the self-adjointness of $A_{\delta',\beta}$ and provides a factorization for the resolvent difference of $A_{\delta',\beta}$ and $A_{N,i,e}$ via Krein's formula
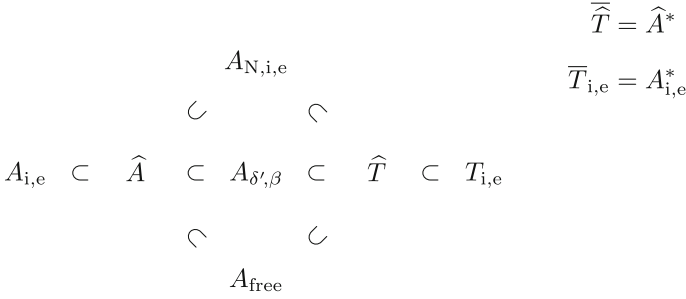
$$\overline{\widehat{T}} = \widehat{A}^*$$

$$A_{\mathrm{N,i,e}}$$

$$\overline{T}_{\mathrm{i,e}} = A_{\mathrm{i,e}}^*$$

$$\curvearrowleft \qquad \curvearrowright$$

$$A_{\mathrm{i,e}} \quad \subset \quad \widehat{A} \quad \subset \quad A_{\delta',\beta} \quad \subset \quad \widehat{T} \quad \subset \quad T_{\mathrm{i,e}}$$

$$\curvearrowright \qquad \curvearrowleft$$

$$A_{\mathrm{free}}$$

FIGURE 2. This figure shows how the operator $A_{\delta',\beta}$ is related to the other operators studied in this section. The operators $A_{\mathrm{N,i,e}}, A_{\delta',\beta}$ and A_{free} are self-adjoint

and a variant of the Birman–Schwinger principle. The first item of the next theorem is part of Theorem A in the introduction.

Theorem 3.11. *Let $A_{\delta',\beta}$ be as above and let $A_{\mathrm{N,i,e}}$ be the self-adjoint operator defined in* (3.4). *Let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and the Weyl function associated with the quasi boundary triple $\widehat{\Pi}$ from Proposition* 3.8. *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 $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\mathrm{N,i,e}})$ the following Krein formula holds:*

$$(A_{\delta',\beta} - \lambda)^{-1} - (A_{\mathrm{N,i,e}} - \lambda)^{-1} = \widehat{\gamma}(\lambda)\big(I - \beta^{-1}\widehat{M}(\lambda)\big)^{-1}\beta^{-1}\,\widehat{\gamma}(\overline{\lambda})^*,$$

where $(I - \beta^{-1}\widehat{M}(\lambda))^{-1} \in \mathcal{B}(L^2(\Sigma))$.

(iii) *For all $\lambda \in \mathbb{R}\backslash\sigma(A_{\mathrm{N,i,e}})$ we have*

$$\lambda \in \sigma_p(A_{\delta',\beta}) \quad \Longleftrightarrow \quad 0 \in \sigma_p\big(I - \beta^{-1}\widehat{M}(\lambda)\big)$$

and $\dim\ker(A_{\delta',\beta} - \lambda) = \dim\ker(I - \beta^{-1}\widehat{M}(\lambda))$.

The next theorem gives assumptions on β which ensure that the domain of the self-adjoint operator $A_{\delta',\beta}$ has H^2-regularity. This theorem is the second part of Theorem B in the introduction.

Theorem 3.12. *Let $A_{\delta',\beta}$ be the self-adjoint Schrödinger operator in Definition* 3.10 *and assume, in addition, that the function $\beta\colon \Sigma \to \mathbb{R}$ is such that $1/\beta \in W^{1,\infty}(\Sigma)$. Then $\mathrm{dom}\, A_{\delta',\beta}$ is contained in $H^2(\mathbb{R}^n\backslash\Sigma)$.*

Proof. The proof proceeds as the proof of Theorem 3.6 with $A_{\delta,\alpha}, A_{\mathrm{free}}, \widetilde{T}, \widetilde{\Gamma}_0,$ $\widetilde{\Gamma}_1$ and α replaced by $A_{\delta',\beta}, A_{\mathrm{N,i,e}}, \widehat{T}, \widehat{\Gamma}_0, \widehat{\Gamma}_1$ and β^{-1}, respectively. Instead of the decomposition (3.14) one has to use the decomposition

$$\mathrm{dom}\,\widehat{T} = \mathrm{dom}\, A_{\mathrm{N,i,e}} \,\dot{+}\, \ker(\widehat{T} - \lambda), \qquad \lambda \in \mathbb{C}\backslash\mathbb{R}.$$

$\square$

3.4. Semi-Boundedness and Point Spectra

In this section we show that the self-adjoint operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ are lower semi-bounded, and that in the case $V \equiv 0$ their negative spectra are finite. We recall some preparatory facts on semi-bounded quadratic forms first.

Definition 3.13. 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

$$\kappa_-(\mathfrak{q}) := \sup\big\{\dim F \colon F \text{ linear subspace of } \operatorname{dom}\mathfrak{q}$$
$$\text{such that } \mathfrak{q}[f] < 0 \text{ for all } f \in F\backslash\{0\}\big\}.$$

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 [56, 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 [15, 10.2 Theorem 3]

$$\dim \operatorname{ran} E_A(-\infty, 0) = \kappa_-(\mathfrak{s}_A) = \kappa_-(\overline{\mathfrak{s}_A}). \tag{3.21}$$

In particular, if $\kappa_-(\mathfrak{s}_A)$ is finite, then the self-adjoint operator A has finitely many negative eigenvalues with finite multiplicities.

In the case $V \equiv 0$ we write $-\Delta_{\delta,\alpha}, -\Delta_{\delta',\beta}$ and $-\Delta_{\text{free}}$ instead of $A_{\delta,\alpha}, A_{\delta',\beta}$ and A_{free}. Now we are ready to formulate and prove the main results of this section. The next theorem is part of Theorem A in the introduction. We mention that finiteness of the negative spectrum in the case of δ-potentials on hypersurfaces was also shown in [18] by other methods.

Theorem 3.14. *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) *$\sigma_{\text{ess}}(-\Delta_{\delta,\alpha}) = \sigma_{\text{ess}}(-\Delta_{\delta',\beta}) = [0, \infty)$.*
  (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 4.3 in Sect. 4.2 below the resolvent difference of the self-adjoint operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\text{free}}$ is compact; thus

$$\sigma_{\text{ess}}(-\Delta_{\delta,\alpha}) = \sigma_{\text{ess}}(-\Delta_{\text{free}}) = [0, \infty).$$

Analogously, according to Theorem 4.5 below the resolvent difference of the self-adjoint operators $-\Delta_{\delta',\beta}$ and $-\Delta_{\text{free}}$ is also compact. Hence

$$\sigma_{\text{ess}}(-\Delta_{\delta',\beta}) = \sigma_{\text{ess}}(-\Delta_{\text{free}}) = [0, \infty).$$

(ii) Let us introduce the (in general non-closed) quadratic forms

$$\mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] := \big(-\Delta_{\delta,\alpha}f, f\big), \quad \operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}}) := \operatorname{dom}(-\Delta_{\delta,\alpha}),$$
$$\mathfrak{s}_{-\Delta_{\delta',\beta}}[f] := \big(-\Delta_{\delta',\beta}f, f\big), \quad \operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}}) := \operatorname{dom}(-\Delta_{\delta',\beta}).$$

Applying the first Green's identity (2.20) to these expressions and taking the definitions (3.12), (3.20) of the domains of the operators $-\Delta_{\delta,\alpha}, -\Delta_{\delta',\beta}$ into account we obtain

$$
\begin{aligned}
\mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] &= \left(-\Delta f_{\mathrm{i}}, f_{\mathrm{i}}\right)_{\mathrm{i}} + \left(-\Delta f_{\mathrm{e}}, f_{\mathrm{e}}\right)_{\mathrm{e}} \\
&= \left(\nabla f_{\mathrm{i}}, \nabla f_{\mathrm{i}}\right)_{\mathrm{i}} - \left(\partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_{\Sigma}, f_{\mathrm{i}}|_{\Sigma}\right)_{\Sigma} + \left(\nabla f_{\mathrm{e}}, \nabla f_{\mathrm{e}}\right)_{\mathrm{e}} - \left(\partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_{\Sigma}, f_{\mathrm{e}}|_{\Sigma}\right)_{\Sigma} \\
&= \left(\nabla f, \nabla f\right) - \left(\alpha f|_{\Sigma}, f|_{\Sigma}\right)_{\Sigma}
\end{aligned}
$$

and

$$
\begin{aligned}
\mathfrak{s}_{-\Delta_{\delta',\beta}}[f] &= \left(-\Delta f_{\mathrm{i}}, f_{\mathrm{i}}\right)_{\mathrm{i}} + \left(-\Delta f_{\mathrm{e}}, f_{\mathrm{e}}\right)_{\mathrm{e}} \\
&= \left(\nabla f_{\mathrm{i}}, \nabla f_{\mathrm{i}}\right)_{\mathrm{i}} - \left(\partial_{\nu_{\mathrm{i}}} f_{\mathrm{i}}|_{\Sigma}, f_{\mathrm{i}}|_{\Sigma}\right)_{\Sigma} + \left(\nabla f_{\mathrm{e}}, \nabla f_{\mathrm{e}}\right)_{\mathrm{e}} - \left(\partial_{\nu_{\mathrm{e}}} f_{\mathrm{e}}|_{\Sigma}, f_{\mathrm{e}}|_{\Sigma}\right)_{\Sigma} \\
&= \left(\nabla f, \nabla f\right) + \left(\beta^{-1}(f_{\mathrm{e}}|_{\Sigma} - f_{\mathrm{i}}|_{\Sigma}), f_{\mathrm{i}}|_{\Sigma}\right)_{\Sigma} - \left(\beta^{-1}(f_{\mathrm{e}}|_{\Sigma} - f_{\mathrm{i}}|_{\Sigma}), f_{\mathrm{e}}|_{\Sigma}\right)_{\Sigma} \\
&= \left(\nabla f, \nabla f\right) - \left(\beta^{-1}(f_{\mathrm{e}}|_{\Sigma} - f_{\mathrm{i}}|_{\Sigma}), f_{\mathrm{e}}|_{\Sigma} - f_{\mathrm{i}}|_{\Sigma}\right)_{\Sigma}.
\end{aligned}
$$

For a bounded function $\sigma\colon \Sigma \to \mathbb{R}$ define the quadratic form $\mathfrak{q}_{\sigma}$

$$
\begin{aligned}
\mathfrak{q}_{\sigma}[f] &:= \left(\nabla f, \nabla f\right) - \left(\sigma f_{\mathrm{i}}|_{\Sigma}, f_{\mathrm{i}}|_{\Sigma}\right)_{\Sigma} - \left(\sigma f_{\mathrm{e}}|_{\Sigma}, f_{\mathrm{e}}|_{\Sigma}\right)_{\Sigma}, \\
\operatorname{dom}\mathfrak{q}_{\sigma} &:= H^1(\mathbb{R}^n\backslash\Sigma).
\end{aligned}
$$

It follows from [12, Theorem 6.9] (cf. the proof of Proposition 3.15 below) 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 (3.21), we have $\kappa_-(\mathfrak{q}_{\sigma}) < \infty$. It can easily be checked that

$$
\operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}}) \subset \operatorname{dom}(\mathfrak{q}_{|\alpha|/2}) \quad \text{and} \quad \forall f \in \operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta,\alpha}})\colon \mathfrak{s}_{-\Delta_{\delta,\alpha}}[f] \geq \mathfrak{q}_{|\alpha|/2}[f].
$$

Using the inequality $|a-b|^2 \leq 2(|a|^2 + |b|^2)$ for complex numbers a, b we obtain

$$
\operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}}) \subset \operatorname{dom}(\mathfrak{q}_{2/|\beta|}) \quad \text{and} \quad \forall f \in \operatorname{dom}(\mathfrak{s}_{-\Delta_{\delta',\beta}})\colon \mathfrak{s}_{-\Delta_{\delta',\beta}}[f] \geq \mathfrak{q}_{2/|\beta|}[f].
$$

These observations yield that

$$
\kappa_-\left(\mathfrak{s}_{-\Delta_{\delta,\alpha}}\right) \leq \kappa_-\left(\mathfrak{q}_{|\alpha|/2}\right) < \infty \quad \text{and} \quad \kappa_-\left(\mathfrak{s}_{-\Delta_{\delta',\beta}}\right) \leq \kappa_-\left(\mathfrak{q}_{2/|\beta|}\right) < \infty.
$$

From this and (3.21) it follows that the negative spectra of $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ are finite. $\qquad\square$

In the following proposition the (closed) sesquilinear form $\mathfrak{a}_{\delta',\beta}$ which induces the self-adjoint operator $-\Delta_{\delta',\beta}$ is determined. This was posed as an open problem in [30, 7.2]. Note that, by the first representation theorem, $\mathfrak{a}_{\delta',\beta}$ is the closure of the form

$$
\mathfrak{s}_{-\Delta_{\delta',\beta}}[f, g] = (-\Delta_{\delta',\beta} f, g), \qquad f, g \in \operatorname{dom}(-\Delta_{\delta',\beta}),
$$

defined in the proof of Theorem 3.14. For completeness we mention that Proposition 3.15 extends naturally to the Schrödinger operator $A_{\delta',\beta}$ with non-trivial $V \in L^\infty(\mathbb{R}^n)$ and the corresponding quadratic form.

Proposition 3.15. *The sesquilinear form*

$$\mathfrak{a}_{\delta',\beta}[f,g] := \left(\nabla f, \nabla g\right) - \left(\beta^{-1}(f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma), g_\mathrm{e}|_\Sigma - g_\mathrm{i}|_\Sigma\right)_\Sigma$$

defined for $f, g \in H^1(\mathbb{R}^n \backslash \Sigma)$ *is symmetric, closed and semi-bounded from below. The self-adjoint operator corresponding to* $\mathfrak{a}_{\delta',\beta}$ *is* $-\Delta_{\delta',\beta}$*, i.e.*

$$(-\Delta_{\delta',\beta} f, g) = \mathfrak{a}_{\delta',\beta}[f,g]$$

holds for all $f \in \mathrm{dom}(-\Delta_{\delta',\beta})$ *and* $g \in H^1(\mathbb{R}^n \backslash \Sigma)$*.*

Proof. Since β is a real-valued function, it follows that the form $\mathfrak{a}_{\delta',\beta}$ is symmetric. In order to show that it is closed and semi-bounded, we consider the forms

$$\mathfrak{a}[f,g] := (\nabla f, \nabla g) \quad \text{and} \quad \mathfrak{a}'[f,g] := -\left(\beta^{-1}(f_\mathrm{e}|_\Sigma - f_\mathrm{i}|_\Sigma), g_\mathrm{e}|_\Sigma - g_\mathrm{i}|_\Sigma\right)_\Sigma$$

on $H^1(\mathbb{R}^n \backslash \Sigma)$, so that $\mathfrak{a}_{\delta',\beta} = \mathfrak{a} + \mathfrak{a}'$ holds. Note that $\mathfrak{a}$ 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

$$\|f_\mathrm{i}|_\Sigma\|_\Sigma \le c_t \|f_\mathrm{i}\|_{H^t(\Omega_\mathrm{i})} \le \varepsilon \|f_\mathrm{i}\|_{H^1(\Omega_\mathrm{i})} + C_\mathrm{i}(\varepsilon) \|f_\mathrm{i}\|_{L^2(\Omega_\mathrm{i})} \tag{3.22}$$

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

$$\begin{aligned}
\|f_\mathrm{e}|_\Sigma\|_\Sigma = \|f_{\mathrm{e},1}|_\Sigma\|_\Sigma &\le \|f_{\mathrm{e},1}|_{\partial\Omega_{\mathrm{e},1}}\|_{L^2(\partial\Omega_{\mathrm{e},1})} \\
&\le \varepsilon \|f_{\mathrm{e},1}\|_{H^1(\Omega_{\mathrm{e},1})} + C_\mathrm{e}(\varepsilon)\|f_{\mathrm{e},1}\|_{L^2(\Omega_{\mathrm{e},1})} \\
&\le \varepsilon \|f_\mathrm{e}\|_{H^1(\Omega_\mathrm{e})} + C_\mathrm{e}(\varepsilon)\|f_\mathrm{e}\|_{L^2(\Omega_\mathrm{e})}
\end{aligned} \tag{3.23}$$

holds for all $f_\mathrm{e} \in H^1(\Omega_\mathrm{e})$. The estimates (3.22) and (3.23) yield that the form $\mathfrak{a}'$ is bounded with respect to $\mathfrak{a}$ with form bound < 1, and hence $\mathfrak{a}_{\delta',\beta} = \mathfrak{a} + \mathfrak{a}'$ is closed and semi-bounded by [56, Theorem VI.1.33]. The remaining statement follows from [56, Theorem VI.2.1] and similar arguments as in the proof of Proposition 3.7. $\square$

Items (i) and (ii) in the next theorem are part of Theorem A in the introduction.

Theorem 3.16. *Let* $\alpha, \beta \colon \Sigma \to \mathbb{R}$ *be such that* $\alpha, 1/\beta \in L^\infty(\Sigma)$ *and let* $V \in L^\infty(\mathbb{R}^n)$ *be a real-valued potential. Moreover, let the self-adjoint operators* $A_{\delta,\alpha}, A_{\delta',\beta}$*, and* A_free *be as in* (3.12)*,* (3.20) *and* (3.5)*, respectively. Then the following statements hold.*

(i) $\sigma_\mathrm{ess}(A_{\delta,\alpha}) = \sigma_\mathrm{ess}(A_{\delta',\beta}) = \sigma_\mathrm{ess}(A_\mathrm{free})$*.*

(ii) *Both self-adjoint operators* $A_{\delta,\alpha}$ *and* $A_{\delta',\beta}$ *are lower semi-bounded.*

Proof. (i) The equality of the essential spectra follows from the stability of the essential spectrum under compact perturbations and Theorems 4.3 and 4.5 below.

(ii) By Theorem 3.14 (ii) the operators $-\Delta_{\delta,\alpha}$ and $-\Delta_{\delta',\beta}$ are bounded from below. The operator of multiplication with the function V is bounded and self-adjoint. Thus the operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ are bounded from below.   □

4. Resolvent Power Differences in $\mathfrak{S}_{p,\infty}$-Classes, Existence and Completeness of Wave Operators

In this section we compare the powers of the resolvents of the singularly perturbed self-adjoint Schrödinger operators $A_{\delta,\alpha}$ and $A_{\delta',\beta}$ with the powers of the resolvents of the unperturbed Schrödinger operator A_{free}. This leads to singular value estimates, which have a long tradition in the analysis of elliptic differential operators, cf. [12–14,49,55] and the recent contributions [10,11,52,53,61] for more details. In this section we prove Theorem C and Theorem D from the Introduction in a slightly stronger form.

4.1. Elliptic Regularity and Some Preliminary $\mathfrak{S}_{p,\infty}$-Estimates

In this section we first provide a typical regularity result for the functions $(A_{\text{free}} - \lambda)^{-1}f$ and $(A_{\text{N,i,e}} - \lambda)^{-1}f$ 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 $A_{\delta,\alpha}, A_{\delta',\beta}, A_{\text{free}}$ and $A_{\text{N,i,e}}$. In the next lemma we make use of the local Sobolev spaces $W_{\Sigma}^{k,\infty}(\mathbb{R}^n), W_{\Sigma}^{k,\infty}(\mathbb{R}^n\backslash\Sigma)$ and $H_{\Sigma}^k(\mathbb{R}^n), H_{\Sigma}^k(\mathbb{R}^n\backslash\Sigma)$ defined in Sect. 2.4.

Lemma 4.1. *Let A_{free} and $A_{\text{N,i,e}}$ be the self-adjoint operators from (3.5) and (3.4), respectively, and let $m \in \mathbb{N}_0$. Then the following assertions hold.*

(i) *If $V \in W_{\Sigma}^{m,\infty}(\mathbb{R}^n)$, then, for all $\lambda \in \rho(A_{\text{free}})$ and $k = 0, 1, \ldots, m$,*

$$f \in H_{\Sigma}^k(\mathbb{R}^n) \quad \Longrightarrow \quad (A_{\text{free}} - \lambda)^{-1}f \in H_{\Sigma}^{k+2}(\mathbb{R}^n).$$

(ii) *If $V \in W_{\Sigma}^{m,\infty}(\mathbb{R}^n\backslash\Sigma)$, then, for all $\lambda \in \rho(A_{\text{N,i,e}})$ and $k = 0, 1, \ldots, m$,*

$$f \in H_{\Sigma}^k(\mathbb{R}^n\backslash\Sigma) \quad \Longrightarrow \quad (A_{\text{N,i,e}} - \lambda)^{-1}f \in H_{\Sigma}^{k+2}(\mathbb{R}^n\backslash\Sigma).$$

Proof. We verify only assertion (i); the proof of (ii) is similar and left to the reader. We proceed by induction with respect to k. For $k = 0$ the statement is an immediate consequence of $H_{\Sigma}^0(\mathbb{R}^n) = L^2(\mathbb{R}^n)$ and $\text{dom}\, A_{\text{free}} = H^2(\mathbb{R}^n)$. Suppose now that the implication in (i) is true for some fixed $k < m$ and let $f \in H_{\Sigma}^{k+1}(\mathbb{R}^n)$. Then, in particular, $f \in H_{\Sigma}^k(\mathbb{R}^n)$ and hence

$$u := (A_{\text{free}} - \lambda)^{-1}f \in H_{\Sigma}^{k+2}(\mathbb{R}^n) \subset H_{\Sigma}^{k+1}(\mathbb{R}^n)$$

by assumption. As $k + 1 \leq m$ and $V \in W_{\Sigma}^{m,\infty}(\mathbb{R}^n)$, it follows from (2.17) that $Vu \in H_{\Sigma}^{k+1}(\mathbb{R}^n)$. Therefore $f - Vu \in H_{\Sigma}^{k+1}(\mathbb{R}^n)$, and since the function u satisfies the differential equation

$$-\Delta u - \lambda u = f - Vu \quad \text{in } \mathbb{R}^n$$

standard results on elliptic regularity yield $u \in H_\Sigma^{k+3}(\mathbb{R}^n)$; see, e.g. [62, Theorem 4.18]. □

An application of the previous lemma yields 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 4.2. *Let* A_{free} *and* $A_{\mathrm{N,i,e}}$ *be the self-adjoint operators from* (3.5) *and* (3.4), *respectively, and let* $\widetilde{\gamma}$ *and* $\widehat{\gamma}$ *be the* γ-*fields from Propositions* 3.2 *and* 3.8, *respectively. Then for a fixed* $m \in \mathbb{N}_0$ *the following statements hold.*

(i) *If* $V \in W_\Sigma^{2m,\infty}(\mathbb{R}^n)$, *then, for all* $\lambda, \mu \in \rho(A_{\mathrm{free}})$ *and* $k = 0, 1, \ldots, m$,

    (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* $V \in W_\Sigma^{2m,\infty}(\mathbb{R}^n \backslash \Sigma)$, *then, for all* $\lambda, \mu \in \rho(A_{\mathrm{N,i,e}})$ *and* $k = 0, 1, \ldots, m$,

    (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

$$\mathrm{ran}(A_{\mathrm{free}} - \lambda)^{-1} = \mathrm{dom}\, A_{\mathrm{free}} = H^2(\mathbb{R}^n) \subset H_\Sigma^2(\mathbb{R}^n),$$

we conclude from Lemma 4.1 (i) that the inclusion

$$\mathrm{ran}\big((A_{\mathrm{free}} - \overline{\mu})^{-1}(A_{\mathrm{free}} - \lambda)^{-k}\big) \subset H_\Sigma^{2k+2}(\mathbb{R}^n)$$

holds for all $k = 0, 1, \ldots, m$. Moreover, since by Proposition 3.2 we have $A_{\mathrm{free}} = \widetilde{T} \upharpoonright \ker \widetilde{\Gamma}_0$, Proposition 2.7 (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

$$\mathrm{ran}\big(\widetilde{\gamma}(\mu)^* (A_{\mathrm{free}} - \lambda)^{-k}\big) \subset H^{2k+3/2}(\Sigma) \tag{4.1}$$

by the properties of the trace map $\widetilde{\Gamma}_1$, cf. (2.18). Now the estimates in (a) and (b) follow from (4.1) and Lemma 2.11 with $\mathcal{K} = L^2(\mathbb{R}^n)$, $q_2 = 2k + \frac{3}{2}$ and with $q_1 = 0$ for (a) and $q_1 = 1$ for (b), respectively. The estimate in (c) follows from (a) by taking the adjoint. □

4.2. Resolvent Power Differences for the Pairs $\{A_{\delta,\alpha}, A_{\mathrm{free}}\}$, $\{A_{\delta',\beta}, A_{\mathrm{free}}\}$ and $\{A_{\delta',\beta}, A_{\mathrm{N,i,e}}\}$

In the next theorem we prove $\mathfrak{S}_{p,\infty}$-properties of resolvent power differences for the self-adjoint operators $A_{\delta,\alpha}$ and A_{free}. The theorem and its corollary are parts of Theorems C and D in the introduction.

Theorem 4.3. *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 (3.12) and (3.5), respectively. Assume that $V \in W_\Sigma^{2m-2,\infty}(\mathbb{R}^n)$ for some $m \in \mathbb{N}$. Then*

$$(A_{\delta,\alpha} - \lambda)^{-l} - (A_{\mathrm{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n)\big)$$

for all $l = 1, 2, \ldots, m$ and for all $\lambda \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\mathrm{free}})$.

Proof. We prove the theorem by applying Lemma 2.3. Fix an arbitrary $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$, and let $\widetilde{\gamma}, \widetilde{M}$ be as in Proposition 3.2. By Theorem 3.5 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 4.2 (i) (a) and (c) imply that the assumptions in Lemma 2.3 are satisfied with

$$H = A_{\delta,\alpha}, \quad K = A_{\mathrm{free}}, \quad B = \widetilde{\gamma}(\lambda_0), \quad C = \big(I - \alpha\widetilde{M}(\lambda_0)\big)^{-1}\alpha\widetilde{\gamma}(\overline{\lambda}_0)^*,$$

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

Since $b = b_1 + b_2 - a = \frac{1}{n-1}$, Lemma 2.3 implies the assertion of the theorem. $\qquad\square$

The previous theorem has a direct application in mathematical scattering theory. Consider the pair $\{A_{\delta,\alpha}, A_{\mathrm{free}}\}$ of self-adjoint operators as a scattering system; here A_{free} stands for the unperturbed operator and $A_{\delta,\alpha}$ is singularly perturbed by a δ-potential of strength α supported on the hypersurface Σ. It is well known (see, e.g. [56, Theorem X.4.8]) that if, for some $m \in \mathbb{N}$, the difference of the mth powers of the resolvents of $A_{\delta,\alpha}$ and A_{free} is a trace class operator, i.e. if

$$(A_{\delta,\alpha} - \lambda_0)^{-m} - (A_{\mathrm{free}} - \lambda_0)^{-m} \in \mathfrak{S}_1$$

for some $\lambda_0 \in \rho(A_{\delta,\alpha}) \cap \rho(A_{\mathrm{free}})$, then the corresponding wave operators

$$W_\pm(A_{\delta,\alpha}, A_{\mathrm{free}}) := \operatorname*{s-lim}_{t\to\pm\infty} e^{itA_{\delta,\alpha}} e^{-itA_{\mathrm{free}}} P_{\mathrm{ac}}(A_{\mathrm{free}})$$

exist and are complete, i.e. the strong limit exists everywhere and the ranges coincide with the absolutely continuous subspace of the perturbed operator $A_{\delta,\alpha}$. Here $P_{\mathrm{ac}}(A_{\mathrm{free}})$ denotes the orthogonal projection onto the absolutely continuous subspace of the unperturbed operator A_{free}. This implies, in particular, that the absolutely continuous parts of $A_{\delta,\alpha}$ and A_{free} are unitarily equivalent and that the absolutely continuous spectra coincide: $\sigma_{\mathrm{ac}}(A_{\delta,\alpha}) = \sigma_{\mathrm{ac}}(A_{\mathrm{free}})$, cf. [56, Theorem X.4.12, Remark X.4.13] and [65,72].

The next corollary shows that for sufficiently smooth potentials V the wave operators of the scattering system $\{A_{\delta,\alpha}, A_{\mathrm{free}}\}$ exist in any space dimension.

Corollary 4.4. *Let the assumptions be as in Theorem 4.3. If $V \in W_\Sigma^{k,\infty}(\mathbb{R}^n)$ for some even k and $k > n - 4$, then the wave operators $W_\pm(A_{\delta,\alpha}, A_{\mathrm{free}})$ exist*

and are complete, and hence the absolutely continuous parts of $A_{\delta,\alpha}$ and A_{free} are unitarily equivalent.

In particular, if $V = 0$, then $W_{\pm}(A_{\delta,\alpha}, A_{\text{free}})$ exist and are complete for any $n \geq 2$ and $\sigma_{\text{ac}}(A_{\delta,\alpha}) = [0, \infty)$.

In the next theorem we prove $\mathfrak{S}_{p,\infty}$-properties for resolvent power differences of the self-adjoint operators $A_{\delta',\beta}$ and A_{free}. The theorem and its corollary are the second parts of Theorems C and D in the introduction. The formulation given below is a bit stronger than the one in the introduction.

Theorem 4.5. *Let β be a real-valued function on Σ such that $1/\beta \in L^{\infty}(\Sigma)$, and let $A_{\delta',\beta}$ and A_{free} be the self-adjoint operators defined in (3.20) and (3.5), respectively. Assume that $V \in W_{\Sigma}^{2m-2,\infty}(\mathbb{R}^n \backslash \Sigma)$ for some $m \in \mathbb{N}$. Then*

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\text{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big)$$

for all $l = 1, 2, \ldots, m$ and for all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{free}})$.

Proof. First we apply Lemma 2.3 to the difference of the lth powers of the resolvents of A_{free} and $A_{\text{N,i,e}}$. Fix an arbitrary $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$ and let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and Weyl function associated with the quasi boundary triple in Proposition 3.8. Since the operators A_{free} and $A_{\text{N,i,e}}$ are both self-adjoint, in analogy to (2.16) we have

$$(A_{\text{free}} - \lambda_0)^{-1} - (A_{\text{N,i,e}} - \lambda_0)^{-1} = -\widehat{\gamma}(\lambda_0)\widehat{M}(\lambda_0)^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*;$$

see [11, Corollary 3.11]. Furthermore, by Proposition 2.7 (v) and Proposition 3.8 (iii) the operator $\widehat{M}(\lambda_0)$ is bijective and closed as an operator from $L^2(\Sigma)$ onto $H^1(\Sigma)$. Hence $\text{dom}\,\widehat{M}(\lambda_0)^{-1} = H^1(\Sigma)$ and $\widehat{M}(\lambda_0)^{-1}$ is closed as an operator from $H^1(\Sigma)$ into $L^2(\Sigma)$. Thus, we can conclude that $\widehat{M}(\lambda_0)^{-1} \in \mathcal{B}(H^1(\Sigma), L^2(\Sigma))$. Set

$$H := A_{\text{free}}, \quad K := A_{\text{N,i,e}}, \quad B := -\widehat{\gamma}(\lambda_0), \quad C := \widehat{M}(\lambda_0)^{-1}\widehat{\gamma}(\overline{\lambda}_0)^*.$$

Then Proposition 4.2 (ii) (b) and (c) imply that the assumptions in Lemma 2.3 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 2.3 implies that

$$(A_{\text{free}} - \lambda)^{-l} - (A_{\text{N,i,e}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big) \tag{4.2}$$

for all $\lambda \in \rho(A_{\text{free}}) \cap \rho(A_{\text{N,i,e}})$ and all $l = 1, 2, \ldots, m$. This observation together with Theorem 4.8 shows that

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\text{free}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l},\infty}\big(L^2(\mathbb{R}^n)\big) \tag{4.3}$$

for all $l = 1, 2, \ldots, m$ and for all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{free}}) \cap \rho(A_{\text{N,i,e}})$. As the resolvent power difference in (4.3) is analytic in λ, it follows that (4.3) holds also for those points $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{free}})$ which are isolated eigenvalues of $A_{\text{N,i,e}}$; note that we know already that the essential spectra of $A_{\text{N,i,e}}, A_{\delta',\beta}$ and A_{free} coincide because the relations (4.2) and (4.3) are true at least for non-real λ. $\qquad\square$

Remark 4.6. We note that in (4.2) it is shown that the difference of the mth powers of the resolvents of A_{free} and $A_{\text{N,i,e}}$ belongs to the class $\mathfrak{S}_{\frac{n-1}{2m},\infty}$ provided $V \in W^{2m-2,\infty}_{\Sigma}(\mathbb{R}^n\backslash\Sigma)$. This is a slight improvement of a result in [12]. For infinitely smooth V the asymptotics of the singular values have been studied in [13,14] and [49].

The following corollary is the counterpart of Corollary 4.4 for the scattering system $\{A_{\delta',\beta}, A_{\text{free}}\}$.

Corollary 4.7. *Let the assumptions be as in Theorem 4.5. If $V \in W^{k,\infty}_{\Sigma}(\mathbb{R}^n\backslash\Sigma)$ for some even k and $k > n-3$, then the wave operators $W_{\pm}(A_{\delta',\beta}, A_{\text{free}})$ exist and are complete, and hence the absolutely continuous parts of $A_{\delta',\beta}$ and A_{free} are unitarily equivalent.*

In particular, if $V = 0$, then $W_{\pm}(A_{\delta',\beta}, A_{\text{free}})$ exist and are complete for any $n \geq 2$ and $\sigma_{\text{ac}}(A_{\delta',\beta}) = [0,\infty)$.

The next result on the $\mathfrak{S}_{p,\infty}$-properties of the resolvent power differences of $A_{\delta',\beta}$ and $A_{\text{N,i,e}}$ completes the proof of Theorem 4.5, but is also of independent interest. We do not formulate the corresponding corollary for the scattering system $\{A_{\delta',\beta}, A_{\text{N,i,e}}\}$.

Theorem 4.8. *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 (3.20) and (3.4), respectively. Assume that $V \in W^{2m-2,\infty}_{\Sigma}(\mathbb{R}^n\backslash\Sigma)$ for some $m \in \mathbb{N}$. Then*

$$(A_{\delta',\beta} - \lambda)^{-l} - (A_{\text{N,i,e}} - \lambda)^{-l} \in \mathfrak{S}_{\frac{n-1}{2l+1},\infty}\big(L^2(\mathbb{R}^n)\big)$$

for all $l = 1, 2, \ldots, m$ and all $\lambda \in \rho(A_{\delta',\beta}) \cap \rho(A_{\text{N,i,e}})$.

Proof. As in the proofs of Theorems 4.3 and 4.5 fix $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$ and let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and Weyl function associated with the quasi boundary triple in Proposition 3.8. By Theorem 3.11 the resolvent difference of $A_{\delta',\beta}$ and $A_{\text{N,i,e}}$ at the point λ_0 can be written in the form

$$(A_{\delta',\beta} - \lambda_0)^{-1} - (A_{\text{N,i,e}} - \lambda_0)^{-1} = \widehat{\gamma}(\lambda_0)\big(I - \beta^{-1}\widehat{M}(\lambda_0)\big)^{-1}\beta^{-1}\widehat{\gamma}(\overline{\lambda_0})^*,$$

where $(I - \beta^{-1}\widehat{M}(\lambda_0))^{-1}\beta^{-1} \in \mathcal{B}(L^2(\Sigma))$. Proposition 4.2 (ii) (a) and (c) imply that the assumptions in Lemma 2.3 are satisfied with

$$H = A_{\delta',\beta}, \quad K = A_{\text{N,i,e}}, \quad B = \widehat{\gamma}(\lambda_0), \quad C = \big(I - \beta^{-1}\widehat{M}(\lambda_0)\big)^{-1}\beta^{-1}\widehat{\gamma}(\overline{\lambda_0})^*,$$
$$a = \frac{2}{n-1}, \quad b_1 = b_2 = \frac{3/2}{n-1}, \quad r = m.$$

Since $b = b_1 + b_2 - a = \frac{1}{n-1}$, Lemma 2.3 implies the assertion of the theorem. $\qquad\square$

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