

Boundary triples for Schrödinger operators with singular interactions on hypersurfaces

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The self-adjoint Schrödinger operator $A_{\delta,\alpha}$ with a δ -interaction of constant strength α supported on a compact smooth hypersurface \mathcal{C} is viewed as a self-adjoint extension of a natural underlying symmetric operator S in $L^2(\mathbb{R}^n)$. The aim of this note is to construct a boundary triple for S^* and a self-adjoint parameter $\Theta_{\delta,\alpha}$ in the boundary space $L^2(\mathcal{C})$ such that $A_{\delta,\alpha}$ corresponds to the boundary condition induced by $\Theta_{\delta,\alpha}$. As a consequence, the well-developed theory of boundary triples and their Weyl functions can be applied. This leads, in particular, to a Krein-type resolvent formula and a description of the spectrum of $A_{\delta,\alpha}$ in terms of the Weyl function and $\Theta_{\delta,\alpha}$.

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1. Introduction

Boundary triples and their Weyl functions are efficient and frequently used tools in the extension theory of symmetric operators and the spectral analysis of their self-adjoint extensions. Roughly speaking, a boundary triple consists of two boundary mappings that satisfy an abstract second Green's identity and a maximality condition. With the help of a boundary triple, all self-adjoint extensions of a symmetric operator can be parameterized via abstract boundary conditions that involve a self-adjoint parameter in a boundary space. In addition, the spectral properties of these self-adjoint extensions can be described with the help of the Weyl function and the corresponding boundary parameters. We refer the reader to [1–5] and Section 2 for more details on boundary triples and their Weyl functions.

The main objective of this note is to provide and discuss boundary triples and their Weyl functions for self-adjoint Schrödinger operators in $L^2(\mathbb{R}^n)$ with δ -interactions of strength $\alpha \in \mathbb{R}$ supported on a compact smooth hypersurface \mathcal{C} that separates \mathbb{R}^n into a smooth bounded domain Ω_i and an unbounded smooth exterior domain Ω_e . In an informal way, such an operator is often written in the form

$$A_{\delta,\alpha} = -\Delta - \alpha\delta_{\mathcal{C}}, \quad (1)$$

where $\delta_{\mathcal{C}}$ denotes the δ -distribution supported on \mathcal{C} . A precise definition of the self-adjoint operator $A_{\delta,\alpha}$ in terms of boundary or interface conditions is given at the beginning of Section 3 below; see also [6, 7] for an equivalent definition via quadratic forms. Schrödinger operators with δ -interactions are frequently used in mathematical physics to model interactions of quantum particles; we refer to the monographs [8] and [9], to the review article [10] and to [6, 11–25] for a small selection of related papers on spectral analysis of such operators.

Let A_{free} be the usual self-adjoint realization of $-\Delta$ in $L^2(\mathbb{R}^n)$ and let $A_{\delta,\alpha}$ be the self-adjoint operator with δ -interaction on \mathcal{C} in (1). We consider the densely defined, closed symmetric operator $S = A_{\text{free}} \cap A_{\delta,\alpha}$ in $L^2(\mathbb{R}^n)$ and its adjoint S^* , and we construct a boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ for S^* and a self-adjoint parameter $\Theta_{\delta,\alpha}$ in $L^2(\mathcal{C})$ such that

$$A_{\text{free}} = S^* \upharpoonright \ker \Gamma_0 \quad \text{and} \quad A_{\delta,\alpha} = S^* \upharpoonright \ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0).$$

Although it is clear from the general theory that such a boundary triple and a self-adjoint parameter $\Theta_{\delta,\alpha}$ exist, its construction is not trivial. Our idea here is based on a coupling of two boundary triples for elliptic PDEs which involve the Dirichlet-to-Neumann map as a regularization (see [26–28]), the restriction of this coupling to a suitable intermediate extension, and certain transforms of boundary triples and corresponding parameters. These efforts and technical considerations are worthwhile for various reasons. In particular, if γ and M denote the γ -field and Weyl function corresponding to the boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ (see Section 2 for more details), then it follows immediately from the general theory in [3,4] that the resolvent difference of A_{free} and $A_{\delta,\alpha}$ admits the representation

$$(A_{\delta,\alpha} - \lambda)^{-1} - (A_{\text{free}} - \lambda)^{-1} = \gamma(\lambda)(\Theta_{\delta,\alpha} - M(\lambda))^{-1}\gamma(\bar{\lambda})^*$$

for all $\lambda \in \rho(A_{\delta,\alpha})$ and belongs to some operator ideal in $L^2(\mathbb{R}^n)$ if and only if the resolvent of $\Theta_{\delta,\alpha}$ belongs to the analogous operator ideal in $L^2(\mathcal{C})$; see Theorem 3.5. As a special case, the Schatten–von Neumann properties of the resolvent difference of A_{free} and $A_{\delta,\alpha}$ carry over to the resolvent of $\Theta_{\delta,\alpha}$, and vice versa. Moreover, the spectral properties of $A_{\delta,\alpha}$ can be described with the help of the perturbation term $(\Theta_{\delta,\alpha} - M(\lambda))^{-1}$. We mention that in the context of the more general notion of quasi boundary triples and their Weyl functions from [29,30] a similar approach as in this note and closely related results can be found in [6,31]; we also refer to [27,28,32–37] for other methods in extension theory of elliptic differential operators.

2. Boundary triples and Weyl functions

In this preparatory section, we recall the notion of boundary triples, associated γ -fields and Weyl functions, and discuss some of their properties. For a more detailed exposition, we refer the reader to [1–5,38].

In the following, let \mathfrak{H} be a Hilbert space, let S be a densely defined, closed symmetric operator in \mathfrak{H} , and let S^* be the adjoint operator.

Definition 2.1. *A triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is called a boundary triple for S^* if \mathcal{G} is a Hilbert space and $\Gamma_0, \Gamma_1 : \text{dom } S^* \rightarrow \mathcal{G}$ are linear mappings that satisfy the abstract second Green’s identity*

$$(S^*f, g)_{\mathfrak{H}} - (f, S^*g)_{\mathfrak{H}} = (\Gamma_1f, \Gamma_0g)_{\mathcal{G}} - (\Gamma_0f, \Gamma_1g)_{\mathcal{G}}$$

for all $f, g \in \text{dom } S^*$, and the mapping $\Gamma := (\Gamma_0, \Gamma_1)^{\top} : \text{dom } S^* \rightarrow \mathcal{G} \times \mathcal{G}$ is surjective.

Recall that a boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for S^* exists if and only if the defect numbers of S coincide or, equivalently, S admits self-adjoint extensions in \mathfrak{H} . Moreover, a boundary triple is not unique (except in the trivial case $S = S^*$). The following special observation will be used in Section 3: suppose that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a boundary triple for S^* and let G be a bounded self-adjoint operator in \mathcal{G} ; then $\{\mathcal{G}, \Gamma'_0, \Gamma'_1\}$, where

$$\begin{pmatrix} \Gamma'_0 \\ \Gamma'_1 \end{pmatrix} = \begin{pmatrix} I & G \\ 0 & I \end{pmatrix} \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix}, \tag{2}$$

is also a boundary triple for S^* . Recall also that $\text{dom } S = \ker \Gamma_0 \cap \ker \Gamma_1$ and that the mapping

$$\Theta \mapsto A_{\Theta} := S^* \upharpoonright \{f \in \text{dom } S^* : \Gamma f = (\Gamma_0f, \Gamma_1f)^{\top} \in \Theta\} \tag{3}$$

establishes a bijective correspondence between the closed linear subspaces (relations) in $\mathcal{G} \times \mathcal{G}$ and the closed linear extensions $A_\Theta \subset S^*$ of S . In the case when Θ is (the graph of) an operator, the closed extension A_Θ in (3) is given by

$$A_\Theta = S^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0). \tag{4}$$

It is important to note that the identity $(A_\Theta)^* = A_{\Theta^*}$ holds and hence A_Θ in (3)–(4) is self-adjoint in \mathfrak{H} if and only if Θ is self-adjoint in \mathcal{G} . It follows, in particular, that the extension

$$A_0 = S^* \upharpoonright \ker \Gamma_0 \tag{5}$$

is self-adjoint. This extension often plays the role of a fixed extension within the family of self-adjoint extensions of S . We also mention that Θ in (3) is an unbounded operator if and only if the extensions A_0 and A_Θ are disjoint but not transversal, that is,

$$S = A_\Theta \cap A_0 \quad \text{and} \quad A_\Theta \hat{+} A_0 \subsetneq S^*, \tag{6}$$

where $\hat{+}$ denotes the sum of subspaces. Note that this appears only in the case when \mathcal{G} is infinite-dimensional, that is, the defect numbers of S are both infinite.

The next theorem can be found in [39]. Very roughly speaking, it can be regarded as converse to the above considerations. Here, the idea is to start with boundary mappings defined on the domain of some operator T that satisfy the abstract second Green’s identity and some additional conditions, and to conclude that T coincides with the adjoint of the restriction of T to the intersection of the kernels of the boundary mappings. Theorem 2.2 will be used in the proof of Lemma 3.1.

Theorem 2.2. *Let T be a linear operator in \mathfrak{H} , let \mathcal{G} be a Hilbert space and assume that $\Gamma_0, \Gamma_1 : \text{dom } T \rightarrow \mathcal{G}$ are linear mappings that satisfy the following conditions:*

- (i) *there exists a self-adjoint restriction A_0 of T in \mathfrak{H} such that $\text{dom } A_0 \subset \ker \Gamma_0$;*
- (ii) $\text{ran}(\Gamma_0, \Gamma_1)^\top = \mathcal{G} \times \mathcal{G}$;
- (iii) *for all $f, g \in \text{dom } T$ the abstract Green’s identity*

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

holds.

Then $S := T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1)$ is a densely defined, closed, symmetric operator in \mathfrak{H} such that $S^ = T$ and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a boundary triple for S^* with the property $A_0 = S^* \upharpoonright \ker \Gamma_0$.*

In the following, we assume that S is a densely defined, closed, symmetric operator in \mathfrak{H} and that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a boundary triple for S^* . Let $A_0 = S^* \upharpoonright \ker \Gamma_0$ be as in (5) and observe that the following direct sum decomposition of $\text{dom } S^*$ is valid:

$$\text{dom } S^* = \text{dom } A_0 \dot{+} \ker(S^* - \lambda) = \ker \Gamma_0 \dot{+} \ker(S^* - \lambda), \quad \lambda \in \rho(A_0).$$

It follows, in particular, that $\Gamma_0 \upharpoonright \ker(S^* - \lambda)$ is a bijective operator from $\ker(S^* - \lambda)$ onto \mathcal{G} . The inverse is denoted by

$$\gamma(\lambda) = (\Gamma_0 \upharpoonright \ker(S^* - \lambda))^{-1}, \quad \lambda \in \rho(A_0);$$

when viewed as a function $\lambda \mapsto \gamma(\lambda)$ on $\rho(A_0)$, we call γ the γ -field corresponding to the boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. The Weyl function M associated with $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is defined by

$$M(\lambda) = \Gamma_1 \gamma(\lambda) = \Gamma_1 (\Gamma_0 \upharpoonright \ker(S^* - \lambda))^{-1}, \quad \lambda \in \rho(A_0).$$

It can be shown that the values $M(\lambda)$ of the Weyl function M are bounded, everywhere defined operators in \mathcal{G} , that M is a holomorphic function on $\rho(A_0)$ with the properties $M(\lambda) = M(\bar{\lambda})^*$ and that $\text{Im } M(\lambda)$ is uniformly positive for $\lambda \in \mathbb{C}^+$, i.e. M is an operator-valued Nevanlinna or Riesz–Herglotz function that is uniformly strict; see [2].

3. Schrödinger operators with δ -interactions on hypersurfaces

Let $\Omega_i \subset \mathbb{R}^n$, $n \geq 2$, be a bounded domain with C^∞ -smooth boundary $\mathcal{C} = \partial\Omega_i$ and let $\Omega_e = \mathbb{R}^n \setminus \overline{\Omega_i}$ be the corresponding exterior domain with the same C^∞ -smooth boundary $\partial\Omega_e = \mathcal{C}$. In the following, $f_i|_{\mathcal{C}}$ and $f_e|_{\mathcal{C}}$ denote the traces of functions in Ω_i and Ω_e , respectively; if $f_i|_{\mathcal{C}} = f_e|_{\mathcal{C}}$, we also set $f|_{\mathcal{C}} := f_i|_{\mathcal{C}} = f_e|_{\mathcal{C}}$. Moreover, $\partial_{\nu_i} f_i|_{\mathcal{C}}$ and $\partial_{\nu_e} f_e|_{\mathcal{C}}$ denote the traces of their normal derivatives; here we agree that the normal vectors ν_i and ν_e point outwards of the domains, so that, $\nu_i = -\nu_e$.

In the following, let $\alpha \neq 0$ be a real constant and consider the Schrödinger operator with a δ -interaction of strength α supported on \mathcal{C} defined by

$$A_{\delta,\alpha} f = -\Delta f, \quad \text{dom } A_{\delta,\alpha} = \left\{ f = \begin{pmatrix} f_i \\ f_e \end{pmatrix} \in H^2(\Omega_i) \times H^2(\Omega_e), \begin{matrix} f_i|_{\mathcal{C}} = f_e|_{\mathcal{C}}, \\ \alpha f|_{\mathcal{C}} = \partial_{\nu_i} f_i|_{\mathcal{C}} + \partial_{\nu_e} f_e|_{\mathcal{C}} \end{matrix} \right\}. \quad (7)$$

According to [6, Theorem 3.5 and Theorem 3.6] the operator $A_{\delta,\alpha}$ is self-adjoint in $L^2(\mathbb{R}^n)$ and corresponds to the densely defined, closed sesquilinear form

$$\begin{aligned} \mathfrak{a}_{\delta,\alpha}[f, g] &= (\nabla f, \nabla g)_{(L^2(\mathbb{R}^n))^n} - \alpha(f|_{\mathcal{C}}, g|_{\mathcal{C}})_{L^2(\mathcal{C})}, \\ \text{dom } \mathfrak{a}_{\delta,\alpha} &= H^1(\mathbb{R}^n). \end{aligned}$$

Observe that the normal derivatives of the functions in $\text{dom } A_{\delta,\alpha}$ may have a jump at the interface \mathcal{C} or, more precisely, that $f \in \text{dom } A_{\delta,\alpha}$ is contained in $H^2(\mathbb{R}^n)$ if and only if $\partial_{\nu_i} f_i|_{\mathcal{C}} = -\partial_{\nu_e} f_e|_{\mathcal{C}}$. We also recall that the essential spectrum of the operator $A_{\delta,\alpha}$ is $[0, \infty)$ and that the negative spectrum consists of a finite number of eigenvalues of finite multiplicity; see [6, 7]. In the following, we fix some point η such that

$$\eta \in \rho(A_{\delta,\alpha}) \cap (-\infty, 0). \quad (8)$$

In Proposition 3.3 below, we specify a boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ for the adjoint of the densely defined, closed, symmetric operator

$$Sf = -\Delta f, \quad \text{dom } S = \{f \in H^2(\mathbb{R}^n) : f|_{\mathcal{C}} = 0\}, \quad (9)$$

such that the free or unperturbed Schrödinger operator

$$A_{\text{free}} f = -\Delta f, \quad \text{dom } A_{\text{free}} = H^2(\mathbb{R}^n),$$

corresponds to the kernel of the first boundary mapping Γ_0 . Note that the operator $A_{\delta,\alpha}$ in (7) is a self-adjoint extension of S and that the defect numbers $\dim(\text{ran}(S \mp i)^\perp)$ are infinite. Hence, the abstract considerations in Section 2 ensure that there exists a self-adjoint operator or relation $\Theta_{\delta,\alpha}$ such that

$$A_{\delta,\alpha} = S^* \upharpoonright \ker(\Gamma_1 - \Theta_{\delta,\alpha} \Gamma_0). \quad (10)$$

The parameter $\Theta_{\delta,\alpha}$ and further properties of the operator $A_{\delta,\alpha}$ will be discussed in Lemma 3.4 and Theorem 3.5 below.

Some further notations and preparatory results are required before Proposition 3.3 can be stated and proved. Consider the densely defined, closed, symmetric operators

$$S_i f_i = -\Delta f_i, \quad \text{dom } S_i = H_0^2(\Omega_i),$$

and

$$S_e f_e = -\Delta f_e, \quad \text{dom } S_e = H_0^2(\Omega_e),$$

in $L^2(\Omega_i)$ and $L^2(\Omega_e)$, respectively. Their adjoints are given by the maximal operators

$$S_i^* f_i = -\Delta f_i, \quad \text{dom } S_i^* = \{f_i \in L^2(\Omega_i) : -\Delta f_i \in L^2(\Omega_i)\},$$

and

$$S_e^* f_e = -\Delta f_e, \quad \text{dom } S_e^* = \{f_e \in L^2(\Omega_e) : -\Delta f_e \in L^2(\Omega_e)\},$$

where the expressions $-\Delta f_i$ and $-\Delta f_e$ are understood in the sense of distributions. It is important to note that $H^2(\Omega_i)$ and $H^2(\Omega_e)$ are proper subsets of the maximal domains $\text{dom } S_i^*$ and $\text{dom } S_e^*$, respectively, and that the symmetric operator S in (9) is an infinite-dimensional extension of the orthogonal sum $S_i \oplus S_e$, which is also a symmetric operator in $L^2(\mathbb{R}^n) = L^2(\Omega_i) \oplus L^2(\Omega_e)$. Recall from [27, 40] that the trace maps admit continuous extensions to the maximal domains (equipped with the graph norms):

$$\text{dom } S_i^* \ni f_i \mapsto f_i|_{\mathcal{C}} \in H^{-1/2}(\mathcal{C}), \quad \text{dom } S_i^* \ni f_i \mapsto \partial_{\nu_i} f_i|_{\mathcal{C}} \in H^{-3/2}(\mathcal{C}),$$

and

$$\text{dom } S_e^* \ni f_e \mapsto f_e|_{\mathcal{C}} \in H^{-1/2}(\mathcal{C}), \quad \text{dom } S_e^* \ni f_e \mapsto \partial_{\nu_e} f_e|_{\mathcal{C}} \in H^{-3/2}(\mathcal{C}).$$

Furthermore, consider the self-adjoint extensions A_i^D and A_e^D of S_i and S_e , respectively, corresponding to Dirichlet boundary conditions on \mathcal{C} :

$$A_i^D f_i = -\Delta f_i, \quad \text{dom } A_i^D = H_0^1(\Omega_i) \cap H^2(\Omega_i),$$

and

$$A_e^D f_e = -\Delta f_e, \quad \text{dom } A_e^D = H_0^1(\Omega_e) \cap H^2(\Omega_e).$$

Since A_i^D and A_e^D are both non-negative, it is clear that η in (8) belongs to $\rho(A_i^D) \cap \rho(A_e^D)$, and hence, we have the direct sum decompositions

$$\text{dom } S_i^* = \text{dom } A_i^D \dot{+} \ker(S_i^* - \eta) = (H_0^1(\Omega_i) \cap H^2(\Omega_i)) \dot{+} \ker(S_i^* - \eta) \quad (11)$$

and

$$\text{dom } S_e^* = \text{dom } A_e^D \dot{+} \ker(S_e^* - \eta) = (H_0^1(\Omega_e) \cap H^2(\Omega_e)) \dot{+} \ker(S_e^* - \eta). \quad (12)$$

We agree to decompose functions $f_i \in \text{dom } S_i^*$ and $f_e \in \text{dom } S_e^*$ in the form

$$f_i = f_i^D + f_i^\eta \quad \text{and} \quad f_e = f_e^D + f_e^\eta, \quad (13)$$

where $f_i^D \in \text{dom } A_i^D$, $f_i^\eta \in \ker(S_i^* - \eta)$, and $f_e^D \in \text{dom } A_e^D$, $f_e^\eta \in \ker(S_e^* - \eta)$.

In the following, we often make use of the operators

$$\iota = (-\Delta_{\mathcal{C}} + I)^{\frac{1}{4}} \quad \text{and} \quad \iota^{-1} = (-\Delta_{\mathcal{C}} + I)^{-\frac{1}{4}},$$

where $\Delta_{\mathcal{C}}$ denotes the Laplace–Beltrami operator on \mathcal{C} . Both mappings ι and ι^{-1} are regarded as isomorphisms

$$\iota : H^s(\mathcal{C}) \rightarrow H^{s-\frac{1}{2}}(\mathcal{C}) \quad \text{and} \quad \iota^{-1} : H^t(\mathcal{C}) \rightarrow H^{t+\frac{1}{2}}(\mathcal{C})$$

for $s, t \in \mathbb{R}$, and also as operators that establish the duality

$$(\iota\varphi, \iota^{-1}\psi)_{L^2(\mathcal{C})} = \langle \varphi, \psi \rangle_{H^{1/2}(\mathcal{C}) \times H^{-1/2}(\mathcal{C})}$$

for $\varphi \in H^{1/2}(\mathcal{C})$ and $\psi \in H^{-1/2}(\mathcal{C})$, when the spaces $H^{1/2}(\mathcal{C})$ and $H^{-1/2}(\mathcal{C})$ are equipped with the corresponding norms. Note also that ι^{-1} can be viewed as a bounded self-adjoint operator in $L^2(\mathcal{C})$ with $\text{ran } \iota^{-1} = H^{1/2}(\mathcal{C})$ and that ι with domain $\text{dom } \iota = H^{1/2}(\mathcal{C})$ is an unbounded self-adjoint operator in $L^2(\mathcal{C})$ with $0 \in \rho(\iota)$.

Now we have finally collected all necessary notation to state the first lemma.

Lemma 3.1. *Let S be the densely defined, closed, symmetric operator in (9). Then the adjoint S^* of S is given by*

$$S^*f = -\Delta f, \quad \text{dom } S^* = \left\{ f = \begin{pmatrix} f_i \\ f_e \end{pmatrix} \in \text{dom } S_i^* \times \text{dom } S_e^*, f_i|_C = f_e|_C \right\}. \quad (14)$$

Further, let

$$\Upsilon_0 f = \iota^{-1} f|_C \quad \text{and} \quad \Upsilon_1 f = -\iota(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C) \quad (15)$$

for $f = (f_i, f_e)^\top \in \text{dom } S^*$ and with f_i^D, f_e^D as in (13). Then $\{L^2(C), \Upsilon_0, \Upsilon_1\}$ is a boundary triple for S^* with the property $A_i^D \oplus A_e^D = S^* \upharpoonright \ker \Upsilon_0$.

Proof. The assertions in Lemma 3.1 will be proved with the help of Theorem 2.2. To this end, we set

$$Tf = -\Delta f, \quad \text{dom } T = \left\{ f = \begin{pmatrix} f_i \\ f_e \end{pmatrix} \in \text{dom } S_i^* \times \text{dom } S_e^*, f_i|_C = f_e|_C \right\},$$

and consider the boundary mappings $\Upsilon_0, \Upsilon_1 : \text{dom } T \rightarrow L^2(C)$ in (15). First of all, we note that item (i) in Theorem 2.2 is satisfied with the self-adjoint operator $A_0 = A_i^D \oplus A_e^D$ since for any function $f = (f_i, f_e)^\top \in \text{dom}(A_i^D \oplus A_e^D) \subset H^2(\Omega_i) \times H^2(\Omega_e)$ one has $f_i \in \text{dom } S_i^*$, $f_e \in \text{dom } S_e^*$, and $f_i|_C = f_e|_C$. In order to see that the mapping

$$\begin{pmatrix} \Upsilon_0 \\ \Upsilon_1 \end{pmatrix} : \text{dom } T \rightarrow L^2(C) \times L^2(C) \quad (16)$$

is surjective, let $\varphi, \psi \in L^2(C)$. Since the Neumann trace map is surjective from $H^2(\Omega_i) \cap H_0^1(\Omega_i)$ onto $H^{1/2}(C)$ and from $H^2(\Omega_e) \cap H_0^1(\Omega_e)$ onto $H^{1/2}(C)$, there exist $f_i^D \in \text{dom } A_i^D$ and $f_e^D \in \text{dom } A_e^D$ such that $\partial_{\nu_i} f_i^D|_C = \partial_{\nu_e} f_e^D|_C = -\frac{1}{2}\iota^{-1}\psi \in H^{1/2}(C)$. Next, we choose $f_i^\eta \in \ker(S_i^* - \eta)$ and $f_e^\eta \in \ker(S_e^* - \eta)$ such that $f_i^\eta|_C = f_e^\eta|_C = \iota\varphi \in H^{-1/2}(C)$, which is possible by the surjectivity of the trace map from the maximal domain onto $H^{-1/2}(C)$; cf. [27, 40, 41]. Now, it is easy to see that $f = (f_i^D + f_i^\eta, f_e^D + f_e^\eta)^\top \in \text{dom } T$ satisfies

$$\Upsilon_0 f = \iota^{-1} f|_C = \varphi \quad \text{and} \quad \Upsilon_1 f = -\iota(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C) = \psi,$$

and hence the map (16) is onto. Next, we verify that the abstract second Green's identity

$$(Tf, g)_{L^2(\mathbb{R}^n)} - (f, Tg)_{L^2(\mathbb{R}^n)} = (\Upsilon_1 f, \Upsilon_0 g)_{L^2(C)} - (\Upsilon_0 f, \Upsilon_1 g)_{L^2(C)}, \quad f, g \in \text{dom } T, \quad (17)$$

holds. For this, it is useful to recall that Green's identity for $f_i = f_i^D + f_i^\eta$ and $g_i = g_i^D + g_i^\eta$ yields

$$\begin{aligned} (S_i^* f_i, g_i)_{L^2(\Omega_i)} - (f_i, S_i^* g_i)_{L^2(\Omega_i)} \\ = \langle f_i|_C, \partial_{\nu_i} g_i^D|_C \rangle_{H^{-1/2}(C) \times H^{1/2}(C)} - \langle \partial_{\nu_i} f_i^D|_C, g_i|_C \rangle_{H^{1/2}(C) \times H^{-1/2}(C)}, \end{aligned} \quad (18)$$

and for $f_e = f_e^D + f_e^\eta$ and $g_e = g_e^D + g_e^\eta$ in the analogous form

$$\begin{aligned} (S_e^* f_e, g_e)_{L^2(\Omega_e)} - (f_e, S_e^* g_e)_{L^2(\Omega_e)} \\ = \langle f_e|_C, \partial_{\nu_e} g_e^D|_C \rangle_{H^{-1/2}(C) \times H^{1/2}(C)} - \langle \partial_{\nu_e} f_e^D|_C, g_e|_C \rangle_{H^{1/2}(C) \times H^{-1/2}(C)}. \end{aligned} \quad (19)$$

Since T is a restriction of the orthogonal sum $S_i^* \oplus S_e^*$ and $f_i|_C = f_e|_C$, $g_i|_C = g_e|_C$ for $f, g \in \text{dom } T$, we conclude from (18) and (19) that

$$\begin{aligned}
& (Tf, g)_{L^2(\mathbb{R}^n)} - (f, Tg)_{L^2(\mathbb{R}^n)} \\
&= (S_i^* f_i, g_i)_{L^2(\Omega_i)} - (f_i, S_i^* g_i)_{L^2(\Omega_i)} + (S_e^* f_e, g_e)_{L^2(\Omega_e)} - (f_e, S_e^* g_e)_{L^2(\Omega_e)} \\
&= \langle f_i|_C, \partial_{\nu_i} g_i^D|_C \rangle_{H^{-1/2}(C) \times H^{1/2}(C)} - \langle \partial_{\nu_i} f_i^D|_C, g_i|_C \rangle_{H^{1/2}(C) \times H^{-1/2}(C)} \\
&\quad + \langle f_e|_C, \partial_{\nu_e} g_e^D|_C \rangle_{H^{-1/2}(C) \times H^{1/2}(C)} - \langle \partial_{\nu_e} f_e^D|_C, g_e|_C \rangle_{H^{1/2}(C) \times H^{-1/2}(C)} \\
&= \langle f|_C, \partial_{\nu_i} g_i^D|_C + \partial_{\nu_e} g_e^D|_C \rangle_{H^{-1/2}(C) \times H^{1/2}(C)} - \langle \partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C, g|_C \rangle_{H^{1/2}(C) \times H^{-1/2}(C)} \\
&= (\iota^{-1} f|_C, \iota(\partial_{\nu_i} g_i^D|_C + \partial_{\nu_e} g_e^D|_C))_{L^2(C)} - (\iota(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C), \iota^{-1} g|_C)_{L^2(C)} \\
&= (-\iota(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C), \iota^{-1} g|_C)_{L^2(C)} - (\iota^{-1} f|_C, -\iota(\partial_{\nu_i} g_i^D|_C + \partial_{\nu_e} g_e^D|_C))_{L^2(C)} \\
&= (\Upsilon_1 f, \Upsilon_0 g)_{L^2(C)} - (\Upsilon_0 f, \Upsilon_1 g)_{L^2(C)}
\end{aligned}$$

holds. Thus, (17) is shown and item (iii) in Theorem 2.2 is satisfied. Hence, Theorem 2.2 implies that the symmetric operator

$$\widehat{S} := T \upharpoonright (\ker \Upsilon_0 \cap \ker \Upsilon_1) \quad (20)$$

is densely defined, closed and its adjoint coincides with T . We show that \widehat{S} coincides with the symmetric operator S in (9). Note first that Theorem 2.2 also implies that

$$A_i^D \oplus A_e^D = T \upharpoonright \ker \Upsilon_0. \quad (21)$$

Both operators, S and \widehat{S} , are restrictions of the operator in (21). We now let $f = (f_i, f_e)^\top \in \text{dom}(A_i^D \oplus A_e^D) = \ker \Upsilon_0$. For such f , we have

$$f \in \ker \Upsilon_1 \iff \partial_{\nu_i} f_i|_C + \partial_{\nu_e} f_e|_C = 0 \iff f \in H^2(\mathbb{R}^n) \iff f \in \text{dom } S.$$

Thus, $\widehat{S} = S$. Now, the remaining statements in Lemma 3.1 follow immediately from Theorem 2.2. \square

Next, we specify the Weyl function N and the γ -field ζ corresponding to the boundary triple $\{L^2(C), \Upsilon_0, \Upsilon_1\}$ in Lemma 3.1. It is clear from the definition of Υ_0 that the γ -field acts as follows:

$$\zeta(\lambda) : L^2(C) \rightarrow L^2(\mathbb{R}^n), \quad \varphi \mapsto f_\lambda, \quad \lambda \in \rho(A_i^D) \cap \rho(A_e^D) = \mathbb{C} \setminus [0, \infty),$$

where $f_\lambda = (f_{i,\lambda}, f_{e,\lambda})^\top \in H^2(\Omega_i) \times H^2(\Omega_e)$ satisfies $-\Delta f_{i,\lambda} = \lambda f_{i,\lambda}$, $-\Delta f_{e,\lambda} = \lambda f_{e,\lambda}$ and

$$f_{i,\lambda}|_C = f_{e,\lambda}|_C = \iota\varphi.$$

In order to specify the Weyl function N , we recall the definition of the Dirichlet-to-Neumann maps $\mathcal{D}_i(\lambda)$ and $\mathcal{D}_e(\lambda)$ associated with the Laplacians on Ω_i and Ω_e , respectively. Note first that for $\varphi, \psi \in H^{-1/2}(C)$ and $\lambda \in \rho(A_i^D)$ and $\mu \in \rho(A_e^D)$ the boundary value problems

$$-\Delta f_i = \lambda f_i, \quad f_i|_C = \varphi \quad \text{and} \quad -\Delta f_e = \mu f_e, \quad f_e|_C = \psi$$

admit unique solutions $f_{i,\lambda} \in \text{dom } S_i^*$ and $f_{e,\mu} \in \text{dom } S_e^*$. Hence, the operators

$$\mathcal{D}_{i,-1/2}(\lambda) f_{i,\lambda}|_C = \partial_{\nu_i} f_{i,\lambda}|_C, \quad \text{dom } \mathcal{D}_{i,-1/2}(\lambda) = H^{-1/2}(C), \quad (22)$$

and

$$\mathcal{D}_{e,-1/2}(\mu) f_{e,\mu}|_C = \partial_{\nu_e} f_{e,\mu}|_C, \quad \text{dom } \mathcal{D}_{e,-1/2}(\mu) = H^{-1/2}(C), \quad (23)$$

are well defined, and map $H^{-1/2}(\mathcal{C})$ into $H^{-3/2}(\mathcal{C})$. We have used the index $-1/2$ in the definition of the Dirichlet-to-Neumann maps in (22) and (23) to indicate that their domain is $H^{-1/2}(\mathcal{C})$. For the following, it is important that the restrictions

$$\mathcal{D}_i(\lambda)f_{i,\lambda}|_{\mathcal{C}} = \partial_{\nu_i}f_{i,\lambda}|_{\mathcal{C}}, \quad \text{dom } \mathcal{D}_i(\lambda) = H^1(\mathcal{C}),$$

and

$$\mathcal{D}_e(\mu)f_{e,\mu}|_{\mathcal{C}} = \partial_{\nu_e}f_{e,\mu}|_{\mathcal{C}}, \quad \text{dom } \mathcal{D}_e(\mu) = H^1(\mathcal{C}),$$

of $\mathcal{D}_{i,-1/2}(\lambda)$ and $\mathcal{D}_{e,-1/2}(\mu)$ to $H^1(\mathcal{C})$ are densely defined, closed, unbounded operators in $L^2(\mathcal{C})$ that satisfy

$$\mathcal{D}_i(\lambda)^* = \mathcal{D}_i(\bar{\lambda}) \quad \text{and} \quad \mathcal{D}_e(\mu)^* = \mathcal{D}_e(\bar{\mu})$$

for all $\lambda \in \rho(A_i^D)$ and for all $\mu \in \rho(A_e^D)$, respectively. For $\lambda \in \rho(A_i^D) \cap \rho(A_e^D) = \mathbb{C} \setminus [0, \infty)$, it is convenient to introduce the operators

$$\mathcal{E}_{-1/2}(\lambda) := \mathcal{D}_{i,-1/2}(\lambda) + \mathcal{D}_{e,-1/2}(\lambda) \quad \text{and} \quad \mathcal{E}(\lambda) := \mathcal{D}_i(\lambda) + \mathcal{D}_e(\lambda). \quad (24)$$

Furthermore, the restrictions of $\mathcal{D}_{i,-1/2}(\lambda)$ and $\mathcal{D}_{e,-1/2}(\mu)$ to $H^{3/2}(\mathcal{C})$ will be used. These restrictions are denoted by $\mathcal{D}_{i,3/2}(\lambda)$ and $\mathcal{D}_{e,3/2}(\mu)$, respectively; they map $H^{3/2}(\mathcal{C})$ into $H^{1/2}(\mathcal{C})$, and as above the index $3/2$ is used to indicate that their domain is $H^{3/2}(\mathcal{C})$.

Lemma 3.2. *Let S be the symmetric operator in (9), let $\{L^2(\mathcal{C}), \Upsilon_0, \Upsilon_1\}$ be the boundary triple for S^* in Lemma 3.1 and fix η as in (8). For $\lambda \in \rho(A_i^D) \cap \rho(A_e^D) = \mathbb{C} \setminus [0, \infty)$ the operators $\mathcal{E}_{-1/2}(\lambda)$ in (24) have the property*

$$\text{ran}(\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta)) \subset H^{1/2}(\mathcal{C}) \quad (25)$$

and the Weyl function corresponding to the boundary triple $\{L^2(\mathcal{C}), \Upsilon_0, \Upsilon_1\}$ is given by

$$N(\lambda) = -\iota(\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta))\iota, \quad \lambda \in \mathbb{C} \setminus [0, \infty).$$

Proof. Let $\lambda \in \rho(A_i^D) \cap \rho(A_e^D)$ and let $f_\lambda = (f_{i,\lambda}, f_{e,\lambda}) \in \ker(S^* - \lambda)$. Then $f_{i,\lambda}|_{\mathcal{C}} = f_{e,\lambda}|_{\mathcal{C}}$ and according to (11)–(13) we have

$$f_{i,\lambda} = f_{i,\lambda}^D + f_{i,\lambda}^\eta \quad \text{and} \quad f_{e,\lambda} = f_{e,\lambda}^D + f_{e,\lambda}^\eta,$$

where $f_{i,\lambda}^D \in \text{dom } A_i^D$, $f_{i,\lambda}^\eta \in \ker(S_i^* - \eta)$, $f_{e,\lambda}^D \in \text{dom } A_e^D$ and $f_{e,\lambda}^\eta \in \ker(S_e^* - \eta)$. Hence, it follows with the help of $f_{i,\lambda}|_{\mathcal{C}} = f_{i,\lambda}^\eta|_{\mathcal{C}}$ and $f_{e,\lambda}|_{\mathcal{C}} = f_{e,\lambda}^\eta|_{\mathcal{C}}$, and the definition of the Dirichlet-to-Neumann maps that

$$\begin{aligned} & (\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta))\iota\Upsilon_0f_\lambda \\ &= (\mathcal{D}_{i,-1/2}(\lambda) - \mathcal{D}_{i,-1/2}(\eta) + \mathcal{D}_{e,-1/2}(\lambda) - \mathcal{D}_{e,-1/2}(\eta))f_\lambda|_{\mathcal{C}} \\ &= \mathcal{D}_{i,-1/2}(\lambda)f_{i,\lambda}|_{\mathcal{C}} - \mathcal{D}_{i,-1/2}(\eta)f_{i,\lambda}^\eta|_{\mathcal{C}} + \mathcal{D}_{e,-1/2}(\lambda)f_{e,\lambda}|_{\mathcal{C}} - \mathcal{D}_{e,-1/2}(\eta)f_{e,\lambda}^\eta|_{\mathcal{C}} \\ &= \partial_{\nu_i}f_{i,\lambda}|_{\mathcal{C}} - \partial_{\nu_i}f_{i,\lambda}^\eta|_{\mathcal{C}} + \partial_{\nu_e}f_{e,\lambda}|_{\mathcal{C}} - \partial_{\nu_e}f_{e,\lambda}^\eta|_{\mathcal{C}} \\ &= \partial_{\nu_i}(f_{i,\lambda} - f_{i,\lambda}^\eta)|_{\mathcal{C}} + \partial_{\nu_e}(f_{e,\lambda} - f_{e,\lambda}^\eta)|_{\mathcal{C}} \\ &= \partial_{\nu_i}f_{i,\lambda}^D|_{\mathcal{C}} + \partial_{\nu_e}f_{e,\lambda}^D|_{\mathcal{C}} \end{aligned} \quad (26)$$

and hence

$$-\iota(\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta))\iota\Upsilon_0f_\lambda = -\iota(\partial_{\nu_i}f_{i,\lambda}^D|_{\mathcal{C}} + \partial_{\nu_e}f_{e,\lambda}^D|_{\mathcal{C}}) = \Upsilon_1f_\lambda.$$

Also, the inclusion (25) follows from (26) since $f_{i,\lambda}^D \in H^2(\Omega_i)$ and $f_{e,\lambda}^D \in H^2(\Omega_e)$, and hence, $\partial_{\nu_i}f_{i,\lambda}^D|_{\mathcal{C}} + \partial_{\nu_e}f_{e,\lambda}^D|_{\mathcal{C}} \in H^{1/2}(\mathcal{C})$ in (26), and for any

$$\varphi \in \text{dom } \mathcal{E}_{-1/2}(\lambda) = \text{dom } \mathcal{E}_{-1/2}(\eta) = H^{-1/2}(\mathcal{C}),$$

there exists $f_\lambda = (f_{i,\lambda}, f_{e,\lambda})^\top \in \ker(S^* - \lambda)$ and $f_\eta = (f_{i,\eta}, f_{e,\eta}) \in \ker(S^* - \eta)$ such that

$$f_{i,\lambda}|_C = f_{e,\lambda}|_C = \varphi = f_{i,\eta}|_C = f_{e,\eta}|_C.$$

□

In the following proposition, we provide a boundary triple for S^* such that the operator A_{free} corresponds to the first boundary mapping. For this, we modify the boundary triple in Lemma 3.1 in a suitable manner.

Proposition 3.3. *Let S be the densely defined, closed, symmetric operator in (9) with adjoint S^* in (14), and let $\mathfrak{E}(\eta) = \iota\mathcal{E}(\eta)\iota$. Then, $\mathfrak{E}(\eta)^{-1}$ is a bounded self-adjoint operator in $L^2(\mathcal{C})$ and $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$, where*

$$\Gamma_0 f = \iota^{-1} f|_C + \mathfrak{E}(\eta)^{-1} \iota (\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C) \quad \text{and} \quad \Gamma_1 f = -\iota (\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C), \quad (27)$$

is a boundary triple for S^* with the property $A_{\text{free}} = S^* \upharpoonright \ker \Gamma_0$. For $\lambda \in \mathbb{C} \setminus [0, \infty)$ the Weyl function corresponding to $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ is given by

$$M(\lambda) = -\iota (\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta)) \iota (I + \mathfrak{E}(\eta)^{-1} \iota (\mathcal{E}_{-1/2}(\lambda) - \mathcal{E}_{-1/2}(\eta)) \iota).$$

Proof. First, we show that $\mathfrak{E}(\eta)^{-1} = \iota^{-1} \mathcal{E}(\eta)^{-1} \iota^{-1}$ is a bounded self-adjoint operator in $L^2(\mathcal{C})$. Observe that $\mathcal{E}(\eta) = \mathcal{D}_i(\eta) + \mathcal{D}_e(\eta)$ is injective. In fact, we assume that $\mathcal{E}(\eta)\varphi = 0$ for some $\varphi \in H^1(\mathcal{C})$, $\varphi \neq 0$. Then, there exists $f_\eta = (f_i^\eta, f_e^\eta)^\top \in \ker(S^* - \eta)$ such that $f_\eta|_C = \varphi$ and hence

$$0 = \mathcal{E}(\eta)\varphi = \mathcal{E}(\eta)f_\eta|_C = \mathcal{D}_i(\eta)f_i^\eta|_C + \mathcal{D}_e(\eta)f_e^\eta|_C = \partial_{\nu_i} f_i^\eta|_C + \partial_{\nu_e} f_e^\eta|_C. \quad (28)$$

Together with $f_i^\eta|_C = f_e^\eta|_C$, this implies that $f_\eta \in \text{dom } A_{\text{free}}$ and hence $\ker(A_{\text{free}} - \eta) \neq \{0\}$. This is impossible, as $\eta < 0$. Thus $\mathcal{E}(\eta)$ is injective. It follows from [6, Proposition 3.2 (iii)] that $\mathcal{E}(\eta)$ is surjective. Hence, $\mathcal{E}(\eta)^{-1}$ is a bounded self-adjoint operator in $L^2(\mathcal{C})$. Since ι^{-1} is also a bounded self-adjoint operator in $L^2(\mathcal{C})$, it is clear that $\mathfrak{E}(\eta)^{-1} = \iota^{-1} \mathcal{E}(\eta)^{-1} \iota^{-1}$ is a bounded self-adjoint operator in $L^2(\mathcal{C})$.

Now, let $\{L^2(\mathcal{C}), \Upsilon_0, \Upsilon_1\}$ be the boundary triple in Lemma 3.1. Note that the boundary mappings Γ_0 and Γ_1 in (27) satisfy:

$$\begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix} = \begin{pmatrix} I & -\mathfrak{E}(\eta)^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} \Upsilon_0 \\ \Upsilon_1 \end{pmatrix}.$$

Hence, it follows that $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ is a boundary triple for S^* ; see (2) in Section 2. Again, we let N denote the Weyl function corresponding to the boundary triple $\{L^2(\mathcal{C}), \Upsilon_0, \Upsilon_1\}$. It is not difficult to see that the Weyl function corresponding to $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ is given by

$$M(\lambda) = N(\lambda)(I - \mathfrak{E}(\eta)^{-1}N(\lambda))^{-1}, \quad \lambda \in \mathbb{C} \setminus [0, \infty).$$

Hence, the form of the Weyl function M follows from Lemma 3.2.

It remains to be shown that $A_{\text{free}} = S^* \upharpoonright \ker \Gamma_0$ holds. Assume that for some $f \in \text{dom } S^*$ we have

$$\iota^{-1} f|_C + \mathfrak{E}(\eta)^{-1} \iota (\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C) = 0. \quad (29)$$

As $\ker \mathcal{E}_{-1/2}(\eta) = \{0\}$ (this can be seen as in (28)), this is equivalent to

$$\mathcal{E}_{-1/2}(\eta)f|_C + (\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C) = 0.$$

Furthermore, since

$$\mathcal{E}_{-1/2}(\eta)f|_C = \mathcal{D}_{i,-1/2}(\eta)f_i^\eta|_C + \mathcal{D}_{e,-1/2}(\eta)f_e^\eta|_C = \partial_{\nu_i} f_i^\eta|_C + \partial_{\nu_e} f_e^\eta|_C$$

holds for f decomposed as in (13), we conclude that (29) is equivalent to

$$\partial_{\nu_i} f_i^\eta|_C + \partial_{\nu_e} f_e^\eta|_C + \partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C = 0,$$

which in turn is equivalent to

$$\partial_{\nu_i} f_i|_C + \partial_{\nu_e} f_e|_C = 0.$$

Therefore, $f \in \ker \Gamma_0$ if and only if $f \in \text{dom } A_{\text{free}}$. □

Our next goal is to identify the self-adjoint parameter $\Theta_{\delta,\alpha}$ such that (10) holds with the boundary triple in Proposition 3.3.

Lemma 3.4. *Let S be the densely defined, closed, symmetric operator in (9) with adjoint S^* in (14), and let $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ be the boundary triple in Proposition 3.3. Then*

$$\Theta_{\delta,\alpha} = \iota(\mathcal{D}_{i,3/2}(\eta) + \mathcal{D}_{e,3/2}(\eta) - \alpha)\iota\left(I - \mathfrak{E}(\eta)^{-1}\iota(\mathcal{D}_{i,3/2}(\eta) + \mathcal{D}_{e,3/2}(\eta) - \alpha)\iota\right)^{-1}$$

is an unbounded self-adjoint operator in $L^2(\mathcal{C})$ such that the Schrödinger operator $A_{\delta,\alpha}$ in (7) corresponds to $\Theta_{\delta,\alpha}$, that is,

$$A_{\delta,\alpha} = S^* \upharpoonright \ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0). \tag{30}$$

Proof. We make use of the fact that the boundary triple $\{L^2(\mathcal{C}), \Upsilon_0, \Upsilon_1\}$ in Lemma 3.1 and the boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ in Proposition 3.3 are related via

$$\Gamma_0 = \Upsilon_0 - \mathfrak{E}(\eta)^{-1}\Upsilon_1 \quad \text{and} \quad \Gamma_1 = \Upsilon_1, \tag{31}$$

and we also make use of the operator

$$\Lambda_{\delta,\alpha} = \iota(\mathcal{D}_{i,3/2}(\eta) + \mathcal{D}_{e,3/2}(\eta) - \alpha)\iota, \quad \text{dom } \Lambda_{\delta,\alpha} = H^2(\mathcal{C}). \tag{32}$$

Our first task is to show that

$$A_{\delta,\alpha} = S^* \upharpoonright \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0) \tag{33}$$

holds. In fact, $f \in \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0)$ if and only if $f \in \text{dom } S^*$ and

$$\iota(\mathcal{D}_{i,3/2}(\eta) + \mathcal{D}_{e,3/2}(\eta) - \alpha)f|_C = -\iota(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C),$$

where $f|_C \in \text{dom } \mathcal{D}_{i,3/2}(\eta) = \text{dom } \mathcal{D}_{e,3/2}(\eta) = H^{3/2}(\mathcal{C})$, together with elliptic regularity, also implies that $f = (f_i, f_e)^\top$ with $f_i \in H^2(\Omega_i)$ and $f_e \in H^2(\Omega_e)$. With f decomposed as in (13) we have

$$(\mathcal{D}_{i,3/2}(\eta) + \mathcal{D}_{e,3/2}(\eta) - \alpha)f|_C = \partial_{\nu_i} f_i^\eta|_C + \partial_{\nu_e} f_e^\eta|_C - \alpha f|_C.$$

Therefore, $f \in \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0)$ if and only if $f = (f_i, f_e)^\top \in \text{dom } S^*$ with $f_i \in H^2(\Omega_i)$ and $f_e \in H^2(\Omega_e)$ and

$$\partial_{\nu_i} f_i^\eta|_C + \partial_{\nu_e} f_e^\eta|_C - \alpha f|_C = -(\partial_{\nu_i} f_i^D|_C + \partial_{\nu_e} f_e^D|_C),$$

and the latter can be rewritten in the form

$$\partial_{\nu_i} f_i|_C + \partial_{\nu_e} f_e|_C = \alpha f|_C.$$

We have shown (33), and as $A_{\delta,\alpha}$ is a self-adjoint operator in $L^2(\mathbb{R}^n)$, it follows that $\Lambda_{\delta,\alpha}$ in (32) is an unbounded self-adjoint operator in $L^2(\mathcal{C})$.

Next, we consider the operator

$$\Theta_{\delta,\alpha} = \Lambda_{\delta,\alpha}(I - \mathfrak{E}(\eta)^{-1}\Lambda_{\delta,\alpha})^{-1} \tag{34}$$

on its natural domain; note that $\ker(I - \mathfrak{E}(\eta)^{-1}\Lambda_{\delta,\alpha}) = \{0\}$ as otherwise $\mathfrak{E}(\eta)\varphi = \Lambda_{\delta,\alpha}\varphi$ for some non-trivial $\varphi \in H^2(\mathcal{C})$, which is a contradiction to $\alpha \neq 0$. Now, we assume that

$f \in \ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0)$. Then, (31) and (34) yield

$$\begin{aligned}
\Upsilon_1 f - \Lambda_{\delta,\alpha}\Upsilon_0 f &= \Gamma_1 f - \Lambda_{\delta,\alpha}(\Gamma_0 + \mathfrak{E}(\eta)^{-1}\Upsilon_1) f \\
&= \Gamma_1 f - \Lambda_{\delta,\alpha}(\Gamma_0 + \mathfrak{E}(\eta)^{-1}\Gamma_1) f \\
&= \Gamma_1 f - \Lambda_{\delta,\alpha}(\Gamma_0 + \mathfrak{E}(\eta)^{-1}\Theta_{\delta,\alpha}\Gamma_0) f \\
&= \Gamma_1 f - \Lambda_{\delta,\alpha}(I + \mathfrak{E}(\eta)^{-1}\Lambda_{\delta,\alpha}(I - \mathfrak{E}(\eta)^{-1}\Lambda_{\delta,\alpha})^{-1})\Gamma_0 f \\
&= \Gamma_1 f - \Lambda_{\delta,\alpha}(I - \mathfrak{E}(\eta)^{-1}\Lambda_{\delta,\alpha})^{-1}\Gamma_0 f \\
&= \Gamma_1 f - \Theta_{\delta,\alpha}\Gamma_0 f \\
&= 0,
\end{aligned}$$

and hence $f \in \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0)$. The converse inclusion is shown in the same way and therefore

$$\ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0) = \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0)$$

and thus the extensions

$$S^* \upharpoonright \ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0) \quad \text{and} \quad S^* \upharpoonright \ker(\Upsilon_1 - \Lambda_{\delta,\alpha}\Upsilon_0),$$

coincide. Therefore, (33) implies (30). Since $A_{\delta,\alpha}$ is self-adjoint in $L^2(\mathbb{R}^n)$, it also follows from (30) that $\Theta_{\delta,\alpha}$ is self-adjoint in $L^2(\mathcal{C})$. Moreover, as S in (9) coincides with the intersection of A_{free} and $A_{\delta,\alpha}$, that is, A_{free} and $A_{\delta,\alpha}$ are disjoint, and since A_{free} and $A_{\delta,\alpha}$ are not transversal, one concludes that $\Theta_{\delta,\alpha}$ is an unbounded operator in $L^2(\mathcal{C})$; cf. (6). \square

We are now able to obtain some immediate and important consequences from the previous considerations, well-known results for boundary triples and Weyl functions [3, 4] and the resolvent estimates in [6, 42].

Theorem 3.5. *Let S be the densely defined, closed, symmetric operator in (9) with adjoint S^* in (14), let $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ be the boundary triple in Proposition 3.3 with*

$$A_{\text{free}} = S^* \upharpoonright \ker \Gamma_0,$$

and let γ and M be the γ -field and Weyl function corresponding to $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$. Furthermore, let $\Theta_{\delta,\alpha}$ be as in Lemma 3.4 so that

$$A_{\delta,\alpha} = S^* \upharpoonright \ker(\Gamma_1 - \Theta_{\delta,\alpha}\Gamma_0).$$

Then, the following assertions hold for all $\lambda \notin [0, \infty)$:

- (i) $\lambda \in \sigma_p(A_{\delta,\alpha})$ if and only if $0 \in \sigma_p(\Theta_{\delta,\alpha} - M(\lambda))$;
- (ii) $\lambda \in \rho(A_{\delta,\alpha})$ if and only if $0 \in \rho(\Theta_{\delta,\alpha} - M(\lambda))$;
- (iii) for all $\lambda \in \rho(A_{\delta,\alpha})$ the resolvent formula

$$(A_{\delta,\alpha} - \lambda)^{-1} - (A_{\text{free}} - \lambda)^{-1} = \gamma(\lambda)(\Theta_{\delta,\alpha} - M(\lambda))^{-1}\gamma(\bar{\lambda})^*$$

is valid, and the resolvent difference of $A_{\delta,\alpha}$ and A_{free} belongs to the Schatten-von Neumann ideal $\mathfrak{S}_p(L^2(\mathbb{R}^n))$ for all $p > \frac{n-1}{3}$;

- (iv) for all $\xi \in \rho(\Theta_{\delta,\alpha})$ the operator $(\Theta_{\delta,\alpha} - \xi)^{-1}$ belongs to the Schatten-von Neumann ideal $\mathfrak{S}_p(L^2(\mathcal{C}))$ for all $p > \frac{n-1}{3}$.

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