A spectral shift function for Schrödinger operators with singular interactions

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Abstract. For the pair $(-\Delta, -\Delta - \alpha\delta_{\mathcal{C}})$ of self-adjoint Schrödinger operators in $L^2(\mathbb{R}^n)$ a spectral shift function is determined in an explicit form with the help of (energy parameter dependent) Dirichlet-to-Neumann maps. Here $\delta_{\mathcal{C}}$ denotes a singular δ-potential which is supported on a smooth compact hypersurface $\mathcal{C} \subset \mathbb{R}^n$ and α is a real-valued function on $\mathcal{C}$.

Mathematics Subject Classification (2010). Primary 35J10; Secondary 47A40, 47A55, 47B25, 81Q10.

Keywords. δ-potential, singular interaction, boundary triple, Weyl–Titchmarsh function, Dirichlet-to-Neumann map, trace formula.

1. Introduction

The goal of this paper is to determine a spectral shift function for the pair $(H, H_{\delta,\alpha})$, where $H = -\Delta$ is the usual self-adjoint Laplacian in $L^2(\mathbb{R}^n)$, and $H_{\delta,\alpha} = -\Delta - \alpha\delta_{\mathcal{C}}$ is a singular perturbation of H by a δ-potential of variable real-valued strength $\alpha \in C^1(\mathcal{C})$ supported on some smooth, compact hypersurface $\mathcal{C}$ that splits $\mathbb{R}^n$, $n \geq 2$, into a bounded interior and an unbounded exterior domain. Schrödinger operators with δ-interactions are often used as idealized models of physical systems with short-range potentials; in the simplest case point interactions are considered, but in the last decades also interactions supported on curves and hypersurfaces have attracted a lot of attention, see the monographs [2, 4, 26], the review [22], and, for instance, [3, 5, 9, 12, 13, 18, 23, 24, 25, 27, 35] for a small selection of papers in this area.

It is known from [9] (see also [12]) that for an integer $m > (n/2) - 1$ the m-th power of the resolvents of H and $H_{\delta,\alpha}$ differs by a trace class operator,

$$\big[(H_{\delta,\alpha} - zI_{L^2(\mathbb{R}^n)})^{-m} - (H - zI_{L^2(\mathbb{R}^n)})^{-m}\big] \in \mathfrak{S}_1(L^2(\mathbb{R}^n)). \tag{1.1}$$

Since both operators H and $H_{\delta,\alpha}$ are bounded from below, [38, Theorem 8.9.1, p. 306–307] applies (upon replacing the pair $(H, H_{\delta,\alpha})$ by $(H+CI_{L^2(\mathbb{R}^n)}, H_{\delta,\alpha}+$

$CI_{L^2(\mathbb{R}^n)})$ such that $H + CI_{L^2(\mathbb{R}^n)} \geq I_{L^2(\mathbb{R}^n)}$ and $H_{\delta,\alpha} + CI_{L^2(\mathbb{R}^n)} \geq I_{L^2(\mathbb{R}^n)}$ for some $C > 0$) and there exists a real-valued function $\xi \in L^1_{\mathrm{loc}}(\mathbb{R})$ satisfying

$$\int_{\mathbb{R}} \frac{|\xi(\lambda)|\, d\lambda}{(1+|\lambda|)^{m+1}} < \infty$$

such that the trace formula

$$\operatorname{tr}_{L^2(\mathbb{R}^n)}\big((H_{\delta,\alpha} - zI_{L^2(\mathbb{R}^n)})^{-m} - (H - zI_{L^2(\mathbb{R}^n)})^{-m}\big) = -m \int_{\mathbb{R}} \frac{\xi(\lambda)\, d\lambda}{(\lambda - z)^{m+1}}$$

is valid for all $z \in \rho(H_{\delta,\alpha}) \cap \rho(H)$. The function ξ in the integrand on the right-hand side is called a *spectral shift function* of the pair $(H, H_{\delta,\alpha})$. For more details, the history and developments of the spectral shift function we refer the reader to the survey papers [14, 16, 17], the standard monographs [38, 40], the paper [39], and the original works [33, 34] by I. M. Lifshitz, [31, 32] by M. G. Krein.

Our approach in this note is based on techniques from extension theory of symmetric operators and relies on a recent representation result of the spectral shift function in terms of an abstract Weyl–Titchmarsh m-function from [6], which we recall in Section 3 for the convenience of the reader. In our situation this abstract Weyl–Titchmarsh m-function will turn out to be a combination of energy dependent Dirichlet-to-Neumann maps $\mathcal{D}_{\mathrm{i}}(z)$ and $\mathcal{D}_{\mathrm{e}}(z)$ associated to $-\Delta$ on the interior and exterior domain, respectively. More precisely, we shall interpret H and $H_{\delta,\alpha}$ as self-adjoint extensions of the densely defined closed symmetric operator

$$Sf = -\Delta f \quad \operatorname{dom}(S) = \big\{ f \in H^2(\mathbb{R}^n) \,\big|\, f \upharpoonright_{\mathcal{C}} = 0 \big\},$$

and make use of the concept of so-called quasi boundary triples and their Weyl fucntions (see [7, 8]). It will then turn out in Theorem 4.5 that the trace class condition (1.1) is satisfied, and in the special case $\alpha(x) < 0$, $x \in \mathcal{C}$, the function

$$\xi(\lambda) = \sum_{j \in J} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \times \Big(\big(\operatorname{Im}\big(\log\big(\big(\overline{\mathcal{D}_{\mathrm{i}}(\lambda + i\varepsilon) + \mathcal{D}_{\mathrm{e}}(\lambda + i\varepsilon)}\big)^{-1} - \alpha^{-1}\big)\big)\big)\varphi_j, \varphi_j \Big)_{L^2(\mathcal{C})}$$

for a.e. $\lambda \in \mathbb{R}$, is a spectral shift function for the pair $(H, H_{\delta,\alpha})$ such that $\xi(\lambda) = 0$ for $\lambda < 0$; here $(\varphi_j)_{j \in J}$ is an orthonormal basis in $L^2(\mathcal{C})$. For the case that no sign condition on the function α is assumed, a slightly more involved formula for the spectral shift function is provided in Theorem 4.3 and in Corollary 4.4.

Next, we briefly summarize the basic notation used in this paper. Let $\mathcal{G}$, $\mathfrak{H}$, etc., be separable complex Hilbert spaces, $(\cdot,\cdot)_{\mathfrak{H}}$ the scalar product in $\mathfrak{H}$ (linear in the first factor), and $I_{\mathfrak{H}}$ the identity operator in $\mathfrak{H}$. If T is a linear operator mapping (a subspace of) a Hilbert space into another, $\operatorname{dom}(T)$ denotes the domain and $\operatorname{ran}(T)$ is the range of T. The closure of a closable operator S is denoted by $\overline{S}$. The spectrum and resolvent set of a closed linear operator in $\mathfrak{H}$ will be denoted by $\sigma(\cdot)$ and $\rho(\cdot)$, respectively. The Banach space of bounded linear operators in $\mathfrak{H}$ is denoted by $\mathcal{L}(\mathfrak{H})$; in the context of two Hilbert spaces, $\mathfrak{H}_j$, $j=1,2$, we use the analogous abbreviation $\mathcal{L}(\mathfrak{H}_1,\mathfrak{H}_2)$. The p-th Schatten–von Neumann ideal consists of compact operators with singular values in ℓ^p, $p>0$, and is denoted by $\mathfrak{S}_p(\mathfrak{H})$ and $\mathfrak{S}_p(\mathfrak{H}_1,\mathfrak{H}_2)$. For $\Omega\subseteq\mathbb{R}^n$ nonempty, $n\in\mathbb{N}$, we suppress the n-dimensional Lebesgue measure d^nx and use the shorthand notation $L^2(\Omega):=L^2(\Omega;d^nx)$; similarly, if $\partial\Omega$ is sufficiently regular we write $L^2(\partial\Omega):=L^2(\partial\Omega;d^{n-1}\sigma)$, with $d^{n-1}\sigma$ the surface measure on $\partial\Omega$. We also abbreviate $\mathbb{C}_\pm:=\{z\in\mathbb{C}\,|\,\mathrm{Im}(z)\gtrless 0\}$ and $\mathbb{N}_0=\mathbb{N}\cup\{0\}$.

2. Quasi boundary triples and their Weyl functions

In this preliminary section we briefly recall the concept of quasi boundary triples and their Weyl functions from extension theory of symmetric operators, which will be used in the next sections. We refer to [7, 8] for more details on quasi boundary triples and to [19, 20, 21, 29, 37] for the closely related concepts of generalized and ordinary boundary triples.

Throughout this section let $\mathfrak{H}$ be a separable Hilbert space and let S be a densely defined closed symmetric operator in $\mathfrak{H}$.

Definition 2.1. *Let $T\subset S^*$ be a linear operator in $\mathfrak{H}$ such that $\overline{T}=S^*$. A triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is said to be a* quasi boundary triple *for $T\subset S^*$ if $\mathcal{G}$ is a Hilbert space and $\Gamma_0,\Gamma_1:\mathrm{dom}(T)\to\mathcal{G}$ are linear mappings such that the following conditions (i)–(iii) are satisfied:*

(i) *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 for all $f,g\in\mathrm{dom}(T)$.

(ii) *The range of the map $(\Gamma_0,\Gamma_1)^\top:\mathrm{dom}(T)\to\mathcal{G}\times\mathcal{G}$ is dense.*

(iii) *The operator $A_0:=T\upharpoonright\ker(\Gamma_0)$ is self-adjoint in $\mathfrak{H}$.*

The next theorem from [7, 8] contains a sufficient condition for a triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ to be a quasi boundary triple. It will be used in the proof of Theorem 4.3.

Theorem 2.2. *Let $\mathfrak{H}$ and $\mathcal{G}$ be separable Hilbert spaces and let T be a linear operator in $\mathfrak{H}$. Assume that $\Gamma_0,\Gamma_1:\mathrm{dom}(T)\to\mathcal{G}$ are linear mappings such that the following conditions (i)–(iii) hold:*

(i) *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 for all $f,g\in\mathrm{dom}(T)$.

(ii) *The range of $(\Gamma_0,\Gamma_1)^\top:\mathrm{dom}(T)\to\mathcal{G}\times\mathcal{G}$ is dense and $\ker(\Gamma_0)\cap\ker(\Gamma_1)$ is dense in $\mathfrak{H}$.*

(iii) *$T\upharpoonright\ker(\Gamma_0)$ is an extension of a self-adjoint operator A_0.*

Then

$$S := T \upharpoonright \big(\ker(\Gamma_0) \cap \ker(\Gamma_1)\big)$$

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

Next, we recall the definition of the γ-field γ and Weyl function M associated to a quasi boundary triple, which is formally the same as in [20, 21] for the case of ordinary or generalized boundary triples. For this let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for $T \subset S^*$ with $A_0 = T \upharpoonright \ker(\Gamma_0)$. We note that the direct sum decomposition

$$\operatorname{dom}(T) = \operatorname{dom}(A_0) \dot{+} \ker(T - zI_{\mathfrak{H}}) = \ker(\Gamma_0) \dot{+} \ker(T - zI_{\mathfrak{H}})$$

of $\operatorname{dom}(T)$ holds for all $z \in \rho(A_0)$, and hence the mapping $\Gamma_0 \upharpoonright \ker(T - zI_{\mathfrak{H}})$ is injective for all $z \in \rho(A_0)$ and its range coincides with $\operatorname{ran}(\Gamma_0)$.

Definition 2.3. *Let* $T \subset S^*$ *be a linear operator in* $\mathfrak{H}$ *such that* $\overline{T} = S^*$ *and let* $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *be a quasi boundary triple for* $T \subset S^*$ *with* $A_0 = T \upharpoonright \ker(\Gamma_0)$. *The* γ-field γ *and the* Weyl function M *corresponding to* $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *are operator-valued functions on* $\rho(A_0)$ *which are defined by*

$$z \mapsto \gamma(z) := \big(\Gamma_0 \upharpoonright \ker(T - zI_{\mathfrak{H}})\big)^{-1} \text{ and } z \mapsto M(z) := \Gamma_1 \big(\Gamma_0 \upharpoonright \ker(T - zI_{\mathfrak{H}})\big)^{-1}.$$

Various useful properties of the γ-field and Weyl function associated to a quasi boundary triple were provided in [7, 8, 11], see also [19, 20, 21, 37] for the special cases of ordinary and generalized boundary triples. In the following we only recall some properties important for our purposes. We first note that the values $\gamma(z)$, $z \in \rho(A_0)$, of the γ-field are operators defined on the dense subspace $\operatorname{ran}(\Gamma_0) \subset \mathcal{G}$ which map onto $\ker(T - zI_{\mathfrak{H}}) \subset \mathfrak{H}$. The operators $\gamma(z)$, $z \in \rho(A_0)$, are bounded and admit continuous extensions $\overline{\gamma(z)} \in \mathcal{L}(\mathcal{G}, \mathfrak{H})$, the function $z \mapsto \overline{\gamma(z)}$ is analytic on $\rho(A_0)$, and one has

$$\frac{d^k}{dz^k}\overline{\gamma(z)} = k!\,(A_0 - zI_{\mathfrak{H}})^{-k}\overline{\gamma(z)}, \qquad k \in \mathbb{N}_0,\ z \in \rho(A_0).$$

For the adjoint operators $\gamma(z)^* \in \mathcal{L}(\mathfrak{H}, \mathcal{G})$, $z \in \rho(A_0)$, it follows from the abstract Green's identity in Definition 2.1 (i) that

$$\gamma(z)^* = \Gamma_1(A_0 - \overline{z}I_{\mathfrak{H}})^{-1}, \quad z \in \rho(A_0), \tag{2.1}$$

and one has

$$\frac{d^k}{dz^k}\gamma(\overline{z})^* = k!\,\gamma(\overline{z})^*(A_0 - zI_{\mathfrak{H}})^{-k}, \qquad k \in \mathbb{N}_0,\ z \in \rho(A_0). \tag{2.2}$$

The values $M(z)$, $z \in \rho(A_0)$, of the Weyl function M associated to a quasi boundary triple are operators in $\mathcal{G}$ with $\operatorname{dom}(M(z)) = \operatorname{ran}(\Gamma_0)$ and $\operatorname{ran}(M(z)) \subseteq \operatorname{ran}(\Gamma_1)$ for all $z \in \rho(A_0)$. In general, $M(z)$ may be an unbounded operator, which is not necessarily closed, but closable. One can show that $z \mapsto M(z)\varphi$ is holomorphic on $\rho(A_0)$ for all $\varphi \in \operatorname{ran}(\Gamma_0)$ and in the case where the values $M(z)$ are densely defined bounded operators for some and hence for all $z \in \rho(A_0)$, one has

$$\frac{d^k}{dz^k}\overline{M(z)} = k!\,\gamma(\overline{z})^*(A_0 - zI_{\mathfrak{H}})^{-(k-1)}\overline{\gamma(z)}, \quad k \in \mathbb{N},\ z \in \rho(A_0). \tag{2.3}$$

3. A representation formula for the spectral shift function

Let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$ and assume that the closed symmetric operator $S = A \cap B$, that is,

$$Sf = Af = Bf, \quad \mathrm{dom}(S) = \big\{f \in \mathrm{dom}(A) \cap \mathrm{dom}(B) \,|\, Af = Bf\big\}, \tag{3.1}$$

is densely defined. According to [6, Proposition 2.4] there exists a quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ with γ-field γ and Weyl function M such that

$$A = T \upharpoonright \ker(\Gamma_0) \ \text{ and } \ B = T \upharpoonright \ker(\Gamma_1), \tag{3.2}$$

and

$$(B - zI_{\mathfrak{H}})^{-1} - (A - zI_{\mathfrak{H}})^{-1} = -\gamma(z)M(z)^{-1}\gamma(\overline{z})^*, \quad z \in \rho(A) \cap \rho(B). \tag{3.3}$$

Next we recall the main result in the abstract part of [6], in which an explicit expression for a spectral shift function of the pair (A, B) in terms of the Weyl function M is found. We refer the reader to [6, Section 4] for a detailed discussion and the proof of Theorem 3.1. We shall use the logarithm of a boundedly invertible dissipative operator in the formula for the spectral shift function below. Here we define for $K \in \mathcal{L}(\mathcal{G})$ with $\mathrm{Im}(K) \geq 0$ and $0 \in \rho(K)$ the logarithm as

$$\log(K) := -i \int_0^\infty \big[(K + i\lambda I_{\mathcal{G}})^{-1} - (1 + i\lambda)^{-1} I_{\mathcal{G}}\big]\, d\lambda;$$

cf. [28, Section 2] for more details. We only mention that $\log(K) \in \mathcal{L}(\mathcal{G})$ by [28, Lemma 2.6].

Theorem 3.1. *Let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$ and assume that for some $\zeta_0 \in \rho(A) \cap \rho(B) \cap \mathbb{R}$ the sign condition*

$$(A - \zeta_0 I_{\mathfrak{H}})^{-1} \geq (B - \zeta_0 I_{\mathfrak{H}})^{-1} \tag{3.4}$$

holds. Let the closed symmetric operator $S = A \cap B$ in (3.1) *be densely defined and let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple with γ-field γ and Weyl function M such that* (3.2)*, and hence also* (3.3)*, hold. Assume that $M(z_1)$, $M(z_2)^{-1}$ are bounded (not necessarily everywhere defined) operators in $\mathcal{G}$ for some $z_1, z_2 \in \rho(A) \cap \rho(B)$ and that for some $k \in \mathbb{N}_0$, all $p, q \in \mathbb{N}_0$, and all $z \in \rho(A) \cap \rho(B)$,*

$$\left(\frac{d^p}{dz^p}\overline{\gamma(z)}\right)\frac{d^q}{dz^q}\big(M(z)^{-1}\gamma(\overline{z})^*\big) \in \mathfrak{S}_1(\mathfrak{H}), \quad p + q = 2k,$$

$$\left(\frac{d^q}{dz^q}\big(M(z)^{-1}\gamma(\overline{z})^*\big)\right)\frac{d^p}{dz^p}\overline{\gamma(z)} \in \mathfrak{S}_1(\mathcal{G}), \quad p + q = 2k,$$

and

$$\frac{d^j}{dz^j}\overline{M(z)} \in \mathfrak{S}_{(2k+1)/j}(\mathcal{G}), \quad j = 1, \dots, 2k+1.$$

Then the following assertions (i) and (ii) hold:

(i) *The difference of the $(2k+1)$-th power of the resolvents of A and B is a trace class operator, that is,*

$$\big[(B - zI_{\mathfrak{H}})^{-(2k+1)} - (A - zI_{\mathfrak{H}})^{-(2k+1)}\big] \in \mathfrak{S}_1(\mathfrak{H})$$

holds for all $z \in \rho(A) \cap \rho(B)$.

(ii) *For any orthonormal basis $\{\varphi_j\}_{j\in J}$ in $\mathcal{G}$ the function*

$$\xi(\lambda) = \sum_{j\in J} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\big(\mathrm{Im}\,\big(\log\big(\overline{M(\lambda + i\varepsilon)}\big)\big)\varphi_j, \varphi_j\big)_{\mathcal{G}} \ \text{for a.e. } \lambda \in \mathbb{R}$$

is a spectral shift function for the pair (A, B) such that $\xi(\lambda) = 0$ in an open neighborhood of ζ_0; the function ξ does not depend on the choice of the orthonormal basis $(\varphi_j)_{j\in J}$. In particular, the trace formula

$$\begin{aligned} &\mathrm{tr}_{\mathfrak{H}}\big((B - zI_{\mathfrak{H}})^{-(2k+1)} - (A - zI_{\mathfrak{H}})^{-(2k+1)}\big) \\ &\quad = -(2k+1)\int_{\mathbb{R}} \frac{\xi(\lambda)\,d\lambda}{(\lambda - z)^{2k+2}}, \quad z \in \rho(A) \cap \rho(B), \end{aligned}$$

holds.

In the special case $k = 0$ Theorem 3.1 can be reformulated and slightly improved; cf. [6, Corollary 4.2]. Here the essential feature is that the limit $\mathrm{Im}(\log(\overline{M(\lambda + i0)}))$ exists in $\mathfrak{S}_1(\mathcal{G})$ for a.e. $\lambda \in \mathbb{R}$.

Corollary 3.2. *Let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$ and assume that for some $\zeta_0 \in \rho(A) \cap \rho(B) \cap \mathbb{R}$ the sign condition*

$$(A - \zeta_0 I_{\mathfrak{H}})^{-1} \geq (B - \zeta_0 I_{\mathfrak{H}})^{-1}$$

holds. Assume that the closed symmetric operator $S = A \cap B$ in (3.1) is densely defined and let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple with γ-field γ and Weyl function M such that (3.2), and hence also (3.3), hold. Assume that $M(z_1)$, $M(z_2)^{-1}$ are bounded (not necessarily everywhere defined) operators in $\mathcal{G}$ for some $z_1, z_2 \in \rho(A)$ and that $\overline{\gamma(z_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ for some $z_0 \in \rho(A)$. Then the following assertions (i)–(iii) hold:

(i) *The difference of the resolvents of A and B is a trace class operator, that is,*

$$\big[(B - zI_{\mathfrak{H}})^{-1} - (A - zI_{\mathfrak{H}})^{-1}\big] \in \mathfrak{S}_1(\mathfrak{H})$$

holds for all $z \in \rho(A) \cap \rho(B)$.

(ii) $\mathrm{Im}(\log(\overline{M(z)})) \in \mathfrak{S}_1(\mathcal{G})$ *for all $z \in \mathbb{C}\backslash\mathbb{R}$ and the limit*

$$\mathrm{Im}\,\big(\log\big(\overline{M(\lambda + i0)}\big)\big) := \lim_{\varepsilon\downarrow 0} \mathrm{Im}\,\big(\log\big(\overline{M(\lambda + i\varepsilon)}\big)\big)$$

exists for a.e. $\lambda \in \mathbb{R}$ in $\mathfrak{S}_1(\mathcal{G})$.

(*iii*) *The function*

$$\xi(\lambda) = \frac{1}{\pi} \operatorname{tr}_{\mathcal{G}}\big(\operatorname{Im}\big(\log\big(\overline{M(\lambda + i0)}\big)\big)\big) \quad \textit{for a.e. } \lambda \in \mathbb{R}$$

is a spectral shift function for the pair (A, B) *such that* $\xi(\lambda) = 0$ *in an open neighborhood of* ζ_0 *and the trace formula*

$$\operatorname{tr}_{\mathfrak{H}}\big((B - zI_{\mathfrak{H}})^{-1} - (A - zI_{\mathfrak{H}})^{-1}\big) = -\int_{\mathbb{R}} \frac{\xi(\lambda)\, d\lambda}{(\lambda - z)^2}$$

is valid for all $z \in \rho(A) \cap \rho(B)$.

We also recall from [6, Section 4] how the sign condition (3.4) in the assumptions in Theorem 3.1 can be replaced by some weaker comparability condition, which is satisfied in our main application in the next section. Again, let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$ and assume that there exists a self-adjoint operator C in $\mathfrak{H}$ such that

$$(C - \zeta_A I_{\mathfrak{H}})^{-1} \geq (A - \zeta_A I_{\mathfrak{H}})^{-1} \quad \text{and} \quad (C - \zeta_B I_{\mathfrak{H}})^{-1} \geq (B - \zeta_B I_{\mathfrak{H}})^{-1}$$

for some $\zeta_A \in \rho(A) \cap \rho(C) \cap \mathbb{R}$ and some $\zeta_B \in \rho(B) \cap \rho(C) \cap \mathbb{R}$, respectively. Assume that the closed symmetric operators $S_A = A \cap C$ and $S_B = B \cap C$ are both densely defined and choose quasi boundary triples $\{\mathcal{G}_A, \Gamma_0^A, \Gamma_1^A\}$ and $\{\mathcal{G}_B, \Gamma_0^B, \Gamma_1^B\}$ with γ-fields γ_A, γ_B and Weyl functions M_A, M_B for

$$T_A = S_A^* \upharpoonright \big(\operatorname{dom}(A) + \operatorname{dom}(C)\big) \quad \text{and} \quad T_B = S_B^* \upharpoonright \big(\operatorname{dom}(B) + \operatorname{dom}(C)\big)$$

such that

$$C = T_A \upharpoonright \ker(\Gamma_0^A) = T_B \upharpoonright \ker(\Gamma_0^B)$$

and

$$A = T_A \upharpoonright \ker(\Gamma_1^A) \quad \text{and} \quad B = T_B \upharpoonright \ker(\Gamma_1^B)$$

(cf. [6, Proposition 2.4]). Next, assume that for some $k \in \mathbb{N}_0$, the conditions in Theorem 3.1 are satisfied for the γ-fields γ_A, γ_B and the Weyl functions M_A, M_B. Then the difference of the $(2k+1)$-th power of the resolvents of A and C, and the difference of the $(2k+1)$-th power of the resolvents of B and C are trace class operators, and for orthonormal bases $(\varphi_j)_{j \in J}$ in $\mathcal{G}_A$ and $(\psi_\ell)_{\ell \in L}$ in $\mathcal{G}_B$ ($J, L \subseteq \mathbb{N}$ appropriate index sets),

$$\xi_A(\lambda) = \sum_{j \in J} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \big(\operatorname{Im}\big(\log\big(\overline{M_A(\lambda + i\varepsilon)}\big)\big)\varphi_j, \varphi_j\big)_{\mathcal{G}_A} \quad \text{for a.e. } \lambda \in \mathbb{R}$$

and

$$\xi_B(\lambda) = \sum_{\ell \in L} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \big(\operatorname{Im}\big(\log\big(\overline{M_B(\lambda + i\varepsilon)}\big)\big)\psi_\ell, \psi_\ell\big)_{\mathcal{G}_B} \quad \text{for a.e. } \lambda \in \mathbb{R}$$

are spectral shift functions for the pairs (C, A) and (C, B), respectively. It follows for $z \in \rho(A) \cap \rho(B) \cap \rho(C)$ that

$$\begin{aligned}
&\operatorname{tr}_{\mathfrak{H}}\big((B - zI_{\mathfrak{H}})^{-(2k+1)} - (A - zI_{\mathfrak{H}})^{-(2k+1)}\big)\\
&\quad = \operatorname{tr}_{\mathfrak{H}}\big((B - zI_{\mathfrak{H}})^{-(2k+1)} - (C - zI_{\mathfrak{H}})^{-(2k+1)}\big)\\
&\qquad - \operatorname{tr}_{\mathfrak{H}}\big((A - zI_{\mathfrak{H}})^{-(2k+1)} - (C - zI_{\mathfrak{H}})^{-(2k+1)}\big)\\
&\quad = -(2k+1)\int_{\mathbb{R}} \frac{[\xi_B(\lambda) - \xi_A(\lambda)]\, d\lambda}{(\lambda - z)^{2k+2}}
\end{aligned}$$

and

$$\int_{\mathbb{R}} \frac{|\xi_B(\lambda) - \xi_A(\lambda)|\, d\lambda}{(1 + |\lambda|)^{2m+2}} < \infty.$$

Therefore,

$$\xi(\lambda) = \xi_B(\lambda) - \xi_A(\lambda) \text{ for a.e. } \lambda \in \mathbb{R} \tag{3.5}$$

is a spectral shift function for the pair (A, B), and in the special case where $\mathcal{G}_A = \mathcal{G}_B := \mathcal{G}$ and $(\varphi_j)_{j\in J}$ is an orthonormal basis in $\mathcal{G}$, one infers that

$$\xi(\lambda) = \sum_{j\in J} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\Big(\big(\operatorname{Im}\big(\log\big(\overline{M_B(\lambda + i\varepsilon)}\big) - \log\big(\overline{M_A(\lambda + i\varepsilon)}\big)\big)\varphi_j, \varphi_j\Big)_{\mathcal{G}} \tag{3.6}$$

for a.e. $\lambda \in \mathbb{R}$. We emphasize that in contrast to the spectral shift function in Theorem 3.1, here the spectral shift function ξ in (3.5) and (3.6) is not necessarily nonnegative.

4. Schrödinger operators with δ-potentials supported on hypersurfaces

The aim of this section is to determine a spectral shift function for the pair $(H, H_{\delta,\alpha})$, where $H = -\Delta$ is the usual self-adjoint Laplacian in $L^2(\mathbb{R}^n)$, and $H_{\delta,\alpha} = -\Delta - \alpha\delta_{\mathcal{C}}$ is a self-adjoint Schrödinger operator with δ-potential of strength α supported on a compact hypersurface $\mathcal{C}$ in $\mathbb{R}^n$ which splits $\mathbb{R}^n$ in a bounded interior domain and an unbounded exterior domain. Throughout this section we shall assume that the following hypothesis holds.

Hypothesis 4.1. *Let $n \in \mathbb{N}$, $n \geq 2$, and $\Omega_{\rm i}$ be a nonempty, open, bounded interior domain in $\mathbb{R}^n$ with a smooth boundary $\partial\Omega_{\rm i}$ and let $\Omega_{\rm e} = \mathbb{R}^n \backslash \overline{\Omega_{\rm i}}$ be the corresponding exterior domain. The common boundary of the interior domain $\Omega_{\rm i}$ and exterior domain $\Omega_{\rm e}$ will be denoted by $\mathcal{C} = \partial\Omega_{\rm e} = \partial\Omega_{\rm i}$. Furthermore, let $\alpha \in C^1(\mathcal{C})$ be a real-valued function on the boundary $\mathcal{C}$.*

We consider the self-adjoint operators in $L^2(\mathbb{R}^n)$ given by

$$Hf = -\Delta f, \quad \operatorname{dom}(H) = H^2(\mathbb{R}^n)$$

and

$$\begin{aligned}
&H_{\delta,\alpha} f = -\Delta f,\\
&\operatorname{dom}(H_{\delta,\alpha}) = \left\{ f = \begin{pmatrix} f_{\rm i} \\ f_{\rm e} \end{pmatrix} \in H^2(\Omega_{\rm i}) \times H^2(\Omega_{\rm e}) \,\middle|\, \begin{matrix} \gamma_D^{\rm i} f_{\rm i} = \gamma_D^{\rm e} f_{\rm e}, \\ \alpha\gamma_D^{\rm i} f_{\rm i} = \gamma_N^{\rm i} f_{\rm i} + \gamma_N^{\rm e} f_{\rm e} \end{matrix} \right\}.
\end{aligned}$$

Here $f_{\rm i}$ and $f_{\rm e}$ denote the restrictions of a function f on $\mathbb{R}^n$ onto $\Omega_{\rm i}$ and $\Omega_{\rm e}$, and $\gamma_D^{\rm i}$, $\gamma_D^{\rm e}$ and $\gamma_N^{\rm i}$, $\gamma_N^{\rm e}$ are the Dirichlet and Neumann trace operators on $H^2(\Omega_{\rm i})$ and $H^2(\Omega_{\rm e})$, respectively. We note that $H_{\delta,\alpha}$ coincides with the self-adjoint operator associated to the quadratic form

$$\mathfrak{h}_{\delta,\alpha}[f,g] = (\nabla f, \nabla g) - \int_{\mathcal{C}} \alpha(x) f(x) \overline{g(x)}\, d\sigma(x), \quad f,g \in H^1(\mathbb{R}^n),$$

see [9, Proposition 3.7] and [18] for more details. For $c \in \mathbb{R}$ we shall also make use of the self-adjoint operator

$$\begin{aligned} &H_{\delta,c} f = -\Delta f, \\ &\operatorname{dom}(H_{\delta,c}) = \left\{ f = \begin{pmatrix} f_{\rm i} \\ f_{\rm e} \end{pmatrix} \in H^2(\Omega_{\rm i}) \times H^2(\Omega_{\rm e}) \,\middle|\, \begin{matrix} \gamma_D^{\rm i} f_{\rm i} = \gamma_D^{\rm e} f_{\rm e}, \\ c\gamma_D^{\rm i} f_{\rm i} = \gamma_N^{\rm i} f_{\rm i} + \gamma_N^{\rm e} f_{\rm e} \end{matrix} \right\}. \end{aligned}$$

The following lemma will be useful for the $\mathfrak{S}_p$-estimates in the proof of Theorem 4.3.

Lemma 4.2. *Let $X \in \mathcal{L}(L^2(\mathbb{R}^n), H^t(\mathcal{C}))$, and assume that* $\operatorname{ran}(X) \subseteq H^s(\mathcal{C})$ *for some $s > t \geq 0$. Then X is compact and* (*cf.* [10, Lemma 4.7])

$$X \in \mathfrak{S}_r\big(L^2(\mathbb{R}^n), H^t(\mathcal{C})\big) \text{ for all } r > (n-1)/(s-t).$$

Next we define interior and exterior Dirichlet-to-Neumann maps $\mathcal{D}_{\rm i}(z)$ and $\mathcal{D}_{\rm e}(\zeta)$ as operators in $L^2(\mathcal{C})$ for all $z, \zeta \in \mathbb{C}\backslash[0,\infty) = \rho(H)$. One notes that for $\varphi, \psi \in H^1(\mathcal{C})$ and $z, \zeta \in \mathbb{C}\backslash[0,\infty)$, the boundary value problems

$$-\Delta f_{{\rm i},z} = z f_{{\rm i},z}, \quad \gamma_D^{\rm i} f_{{\rm i},z} = \varphi, \tag{4.1}$$

and

$$-\Delta f_{{\rm e},\zeta} = \zeta f_{{\rm e},\zeta}, \quad \gamma_D^{\rm e} f_{{\rm e},\zeta} = \psi, \tag{4.2}$$

admit unique solutions $f_{{\rm i},z} \in H^{3/2}(\Omega_{\rm i})$ and $f_{{\rm e},\zeta} \in H^{3/2}(\Omega_{\rm e})$, respectively. The corresponding solution operators are denoted by

$$P_{\rm i}(z) : L^2(\mathcal{C}) \to L^2(\Omega_{\rm i}), \quad \varphi \mapsto f_{{\rm i},z},$$

and

$$P_{\rm e}(\zeta) : L^2(\mathcal{C}) \to L^2(\Omega_{\rm e}), \quad \psi \mapsto f_{{\rm e},\zeta}.$$

The *interior Dirichlet-to-Neumann map* in $L^2(\mathcal{C})$,

$$\mathcal{D}_{\rm i}(z) : H^1(\mathcal{C}) \to L^2(\mathcal{C}), \quad \varphi \mapsto \gamma_N^{\rm i} P_{\rm i}(z)\varphi, \tag{4.3}$$

maps Dirichlet boundary values $\gamma_D^{\rm i} f_{{\rm i},z}$ of the solutions $f_{{\rm i},z} \in H^{3/2}(\Omega_{\rm i})$ of (4.1) to the corresponding Neumann boundary values $\gamma_N^{\rm i} f_{{\rm i},z}$, and the *exterior Dirichlet-to-Neumann map* in $L^2(\mathcal{C})$,

$$\mathcal{D}_{\rm e}(\zeta) : H^1(\mathcal{C}) \to L^2(\mathcal{C}), \quad \psi \mapsto \gamma_N^{\rm e} P_{\rm e}(\zeta)\psi, \tag{4.4}$$

maps Dirichlet boundary values $\gamma_D^{\rm e} f_{{\rm e},\zeta}$ of the solutions $f_{{\rm e},\zeta} \in H^{3/2}(\Omega_{\rm e})$ of (4.2) to the corresponding Neumann boundary values $\gamma_N^{\rm e} f_{{\rm e},\zeta}$. The interior and exterior Dirichlet-to-Neumann maps are both closed unbounded operators in $L^2(\mathcal{C})$.

In the next theorem a spectral shift function for the pair $(H, H_{\delta,\alpha})$ is expressed in terms of the limits of the sum of the interior and exterior

Dirichlet-to-Neumann map $\mathcal{D}_{\rm i}(z)$ and $\mathcal{D}_{\rm e}(z)$ and the function α. It will turn out that the operators $\mathcal{D}_{\rm i}(z)+\mathcal{D}_{\rm e}(z)$ are boundedly invertible for all $z\in\mathbb{C}\backslash[0,\infty)$ and for our purposes it is convenient to work with the function

$$z\mapsto \mathcal{E}(z)=\big(\mathcal{D}_{\rm i}(z)+\mathcal{D}_{\rm e}(z)\big)^{-1},\quad z\in\mathbb{C}\backslash[0,\infty). \tag{4.5}$$

It was shown in [9, Proposition 3.2 (iii) and Remark 3.3] that $\mathcal{E}(z)$ is a compact operator in $L^2(\mathcal{C})$ which extends the acoustic single layer potential for the Helmholtz equation, that is,

$$(\mathcal{E}(z)\varphi)(x)=\int_{\mathcal{C}}G(z,x,y)\varphi(y)d\sigma(y),\quad x\in\mathcal{C},\ \varphi\in C^\infty(\mathcal{C}),$$

where $G(z,\cdot\,,\cdot\,)$, $z\in\mathbb{C}\backslash[0,\infty)$, represents the integral kernel of the resolvent of H (cf. [36, Chapter 6] and [9, Remark 3.3]). Explicitly,

$$\begin{aligned} G(z,x,y)=(i/4)\big(2\pi z^{-1/2}|x-y|\big)^{(2-n)/2}H^{(1)}_{(n-2)/2}\big(z^{1/2}|x-y|\big),\\ z\in\mathbb{C}\backslash[0,\infty),\ \operatorname{Im}\big(z^{1/2}\big)>0,\ x,y\in\mathbb{R}^n,\ x\neq y,\ n\geqslant 2.\end{aligned}$$

Here $H^{(1)}_\nu(\,\cdot\,)$ denotes the Hankel function of the first kind with index $\nu\geq 0$ (cf. [1, Sect. 9.1]).

We mention that the trace class property of the difference of the $(2k+1)$-th power of the resolvents in the next theorem is known from [9] (see also [12]).

Theorem 4.3. *Assume Hypothesis* 4.1*, let* $\mathcal{E}(z)$ *be defined as in* (4.5)*, let* $\alpha\in C^1(\mathcal{C})$ *be a real-valued function and fix* $c>0$ *such that* $\alpha(x)<c$ *for all* $x\in\mathcal{C}$*. Then the following assertions* (i) *and* (ii) *hold for* $k\in\mathbb{N}_0$ *such that* $k\geq (n-3)/4$*:*

(i) *The difference of the* $(2k+1)$*-th power of the resolvents of* H *and* $H_{\delta,\alpha}$ *is a trace class operator, that is,*

$$\big[(H_{\delta,\alpha}-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}-(H-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big]\in\mathfrak{S}_1\big(L^2(\mathbb{R}^n)\big)$$

holds for all $z\in\rho(H_{\delta,\alpha})=\rho(H)\cap\rho(H_{\delta,\alpha})$.

(ii) *For any orthonormal basis* $(\varphi_j)_{j\in J}$ *in* $L^2(\mathcal{C})$ *the function*

$$\xi(\lambda)=\sum_{j\in J}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\Big(\big(\operatorname{Im}\big(\log(\mathcal{M}_\alpha(\lambda+i\varepsilon))-\log(\mathcal{M}_0(\lambda+i\varepsilon))\big)\big)\varphi_j,\varphi_j\Big)_{L^2(\mathcal{C})}$$

for a.e. $\lambda\in\mathbb{R}$ *with*

$$\mathcal{M}_0(z)=-c^{-1}\big(c\mathcal{E}(z)-I_{L^2(\mathcal{C})}\big)^{-1}, \tag{4.6}$$

$$\mathcal{M}_\alpha(z)=(c-\alpha)^{-1}\big(\alpha\mathcal{E}(z)-I_{L^2(\mathcal{C})}\big)\big(c\mathcal{E}(z)-I_{L^2(\mathcal{C})}\big)^{-1}, \tag{4.7}$$

for $z\in\mathbb{C}\backslash\mathbb{R}$*, is a spectral shift function for the pair* $(H,H_{\delta,\alpha})$ *such that* $\xi(\lambda)=0$ *for* $\lambda<\inf(\sigma(H_{\delta,c}))$ *and the trace formula*

$$\begin{aligned}&\operatorname{tr}_{L^2(\mathbb{R}^n)}\big((H_{\delta,\alpha}-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}-(H-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big)\\ &\qquad\qquad=-(2k+1)\int_{\mathbb{R}}\frac{\xi(\lambda)\,d\lambda}{(\lambda-z)^{2k+2}}\end{aligned}$$

is valid for all $z \in \rho(H_{\delta,\alpha}) = \rho(H) \cap \rho(H_{\delta,\alpha})$.

Proof. The structure and underlying idea of the proof of Theorem 4.3 is as follows. In the first two steps a suitable quasi boundary triple and its Weyl function are constructed. In the third step it is shown that the assumptions in Theorem 3.1 are satisfied.

Step 1. Since $c - \alpha(x) \neq 0$ for all $x \in \mathcal{C}$ by assumption, the closed symmetric operator $S = H_{\delta,c} \cap H_{\delta,\alpha}$ is given by

$$Sf = -\Delta f, \quad \operatorname{dom}(S) = \bigl\{ f \in H^2(\mathbb{R}^n) \,\big|\, \gamma_D^{\mathrm{i}} f_{\mathrm{i}} = \gamma_D^{\mathrm{e}} f_{\mathrm{e}} = 0 \bigr\}.$$

In this step we show that the operator

$$T = -\Delta, \quad \operatorname{dom}(T) = \left\{ f = \begin{pmatrix} f_{\mathrm{i}} \\ f_{\mathrm{e}} \end{pmatrix} \in H^2(\Omega_{\mathrm{i}}) \times H^2(\Omega_{\mathrm{e}}) \,\middle|\, \gamma_D^{\mathrm{i}} f_{\mathrm{i}} = \gamma_D^{\mathrm{e}} f_{\mathrm{e}} \right\},$$

satisfies $\overline{T} = S^*$ and that $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$, where

$$\Gamma_0 f = c\gamma_D^{\mathrm{i}} f_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}), \quad \operatorname{dom}(\Gamma_0) = \operatorname{dom}(T), \tag{4.8}$$

and

$$\Gamma_1 f = \frac{1}{c - \alpha}\bigl(\alpha\gamma_D^{\mathrm{i}} f_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}})\bigr), \quad \operatorname{dom}(\Gamma_1) = \operatorname{dom}(T), \tag{4.9}$$

is a quasi boundary triple for $T \subset S^*$ such that

$$H_{\delta,c} = T \upharpoonright \ker(\Gamma_0) \ \text{ and } \ H_{\delta,\alpha} = T \upharpoonright \ker(\Gamma_1). \tag{4.10}$$

For the proof of this fact we make use of Theorem 2.2 and verify next that assumptions (i)–(iii) in Theorem 2.2 are satisfied with the above choice of S, T and boundary maps Γ_0 and Γ_1. For $f, g \in \operatorname{dom}(T)$ one computes

$$\begin{aligned}
&(\Gamma_1 f, \Gamma_0 g)_{L^2(\mathcal{C})} - (\Gamma_0 f, \Gamma_1 g)_{L^2(\mathcal{C})} \\
&\quad= \Bigl(\tfrac{1}{c-\alpha}\bigl(\alpha\gamma_D^{\mathrm{i}} f_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}})\bigr), c\gamma_D^{\mathrm{i}} g_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}}) \Bigr)_{L^2(\mathcal{C})} \\
&\qquad - \Bigl(c\gamma_D^{\mathrm{i}} f_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}), \tfrac{1}{c-\alpha}\bigl(\alpha\gamma_D^{\mathrm{i}} g_{\mathrm{i}} - (\gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}})\bigr) \Bigr)_{L^2(\mathcal{C})} \\
&\quad= -\bigl(\tfrac{\alpha}{c-\alpha}\gamma_D^{\mathrm{i}} f_{\mathrm{i}}, \gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}} \bigr)_{L^2(\mathcal{C})} - \bigl(\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \tfrac{c}{c-\alpha}\gamma_D^{\mathrm{i}} g_{\mathrm{i}} \bigr)_{L^2(\mathcal{C})} \\
&\qquad + \bigl(\tfrac{c}{c-\alpha}\gamma_D^{\mathrm{i}} f_{\mathrm{i}}, \gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}} \bigr)_{L^2(\mathcal{C})} + \bigl(\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \tfrac{\alpha}{c-\alpha}\gamma_D^{\mathrm{i}} g_{\mathrm{i}} \bigr)_{L^2(\mathcal{C})} \\
&\quad= \bigl(\gamma_D^{\mathrm{i}} f_{\mathrm{i}}, \gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}} \bigr)_{L^2(\mathcal{C})} - \bigl(\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \gamma_D^{\mathrm{i}} g_{\mathrm{i}} \bigr)_{L^2(\mathcal{C})},
\end{aligned}$$

and on the other hand, Green's identity and $\gamma_D^{\mathrm{i}} f_{\mathrm{i}} = \gamma_D^{\mathrm{e}} f_{\mathrm{e}}$ and $\gamma_D^{\mathrm{i}} g_{\mathrm{i}} = \gamma_D^{\mathrm{e}} g_{\mathrm{e}}$ yield

$$\begin{aligned}
&(Tf, g)_{L^2(\mathbb{R}^n)} - (f, Tg)_{L^2(\mathbb{R}^n)} \\
&\quad= (-\Delta f_{\mathrm{i}}, g_{\mathrm{i}})_{L^2(\Omega_{\mathrm{i}})} - (f_{\mathrm{i}}, -\Delta g_{\mathrm{i}})_{L^2(\Omega_{\mathrm{i}})} + (-\Delta f_{\mathrm{e}}, g_{\mathrm{e}})_{L^2(\Omega_{\mathrm{e}})} \\
&\qquad - (f_{\mathrm{e}}, -\Delta g_{\mathrm{e}})_{L^2(\Omega_{\mathrm{e}})} \\
&\quad= (\gamma_D^{\mathrm{i}} f_{\mathrm{i}}, \gamma_N^{\mathrm{i}} g_{\mathrm{i}})_{L^2(\mathcal{C})} - (\gamma_N^{\mathrm{i}} f_{\mathrm{i}}, \gamma_D^{\mathrm{i}} g_{\mathrm{i}})_{L^2(\mathcal{C})} \\
&\qquad + (\gamma_D^{\mathrm{e}} f_{\mathrm{e}}, \gamma_N^{\mathrm{e}} g_{\mathrm{e}})_{L^2(\mathcal{C})} - (\gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \gamma_D^{\mathrm{e}} g_{\mathrm{e}})_{L^2(\mathcal{C})} \\
&\quad= \bigl(\gamma_D^{\mathrm{i}} f_{\mathrm{i}}, \gamma_N^{\mathrm{i}} g_{\mathrm{i}} + \gamma_N^{\mathrm{e}} g_{\mathrm{e}} \bigr)_{L^2(\mathcal{C})} - \bigl(\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \gamma_D^{\mathrm{i}} g_{\mathrm{i}} \bigr)_{L^2(\mathcal{C})},
\end{aligned}$$

and hence condition (i) in Theorem 2.2 holds. Next, in order to show that $\operatorname{ran}(\Gamma_0, \Gamma_1)^\top$ is dense in $L^2(\mathcal{C})$ we recall that

$$\begin{pmatrix} \gamma_D^{\mathrm{i}} \\ \gamma_N^{\mathrm{i}} \end{pmatrix} : H^2(\Omega_{\mathrm{i}}) \to H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C})$$

and

$$\begin{pmatrix} \gamma_D^{\mathrm{e}} \\ \gamma_N^{\mathrm{e}} \end{pmatrix} : H^2(\Omega_{\mathrm{e}}) \to H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C})$$

are surjective mappings. It follows that also the mapping

$$\begin{pmatrix} \gamma_D^{\mathrm{i}} \\ \gamma_N^{\mathrm{i}} + \gamma_N^{\mathrm{e}} \end{pmatrix} : \operatorname{dom}(T) \to H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C}) \tag{4.11}$$

is surjective, and since the 2×2-block operator matrix

$$\Theta := \begin{pmatrix} c I_{L^2(\mathcal{C})} & -I_{L^2(\mathcal{C})} \\ \frac{\alpha}{c-\alpha} I_{L^2(\mathcal{C})} & -\frac{1}{c-\alpha} I_{L^2(\mathcal{C})} \end{pmatrix}$$

is an isomorphism in $L^2(\mathcal{C}) \times L^2(\mathcal{C})$, it follows that the range of the mapping

$$\begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix} = \Theta \begin{pmatrix} \gamma_D^{\mathrm{i}} \\ \gamma_N^{\mathrm{i}} + \gamma_N^{\mathrm{e}} \end{pmatrix} : \operatorname{dom}(T) \to L^2(\mathcal{C}) \times L^2(\mathcal{C}),$$

is dense. Furthermore, as $C_0^\infty(\Omega_{\mathrm{i}}) \times C_0^\infty(\Omega_{\mathrm{e}})$ is contained in $\ker(\Gamma_0) \cap \ker(\Gamma_1)$, it is clear that $\ker(\Gamma_0) \cap \ker(\Gamma_1)$ is dense in $L^2(\mathbb{R}^n)$. Hence one concludes that condition (ii) in Theorem 2.2 is satisfied. Condition (iii) in Theorem 2.2 is satisfied since (4.10) holds by construction and $H_{\delta,c}$ is self-adjoint. Thus, Theorem 2.2 implies that the closed symmetric operator

$$T \upharpoonright \big(\ker(\Gamma_0) \cap \ker(\Gamma_1)\big) = H_{\delta,c} \cap H_{\delta,\alpha} = S$$

is densely defined, its adjoint coincides with $\overline{T}$, and $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $T \subset S^*$ such that (4.10) holds.

Step 2. In this step we prove that for $z \in \rho(H_{\delta,c}) \cap \rho(H)$ the Weyl function corresponding to the quasi boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ is given by

$$\begin{aligned} M(z) &= \frac{1}{c-\alpha} \big(\alpha \mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big) \big(c \mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)^{-1}, \\ \operatorname{dom}(M(z)) &= H^{1/2}(\mathcal{C}), \end{aligned} \tag{4.12}$$

where $\mathcal{E}_{1/2}(z)$ denotes the restriction of the operator $\mathcal{E}(z)$ in (4.5) onto $H^{1/2}(\mathcal{C})$. Furthermore, we verify that $M(z_1)$ and $M(z_2)^{-1}$ are bounded for some $z_1, z_2 \in \mathbb{C}\backslash\mathbb{R}$, and we conclude that the closures of the operators $M(z)$, $z \in \mathbb{C}\backslash\mathbb{R}$, in $L^2(\mathcal{C})$ are given by the operators $\mathcal{M}_\alpha(z)$ in (4.6), (4.7).

It will first be shown that the operator $\mathcal{E}(z)$ and its restriction $\mathcal{E}_{1/2}(z)$ are well-defined for all $z \in \rho(H) = \mathbb{C}\backslash[0,\infty)$. For this fix $z \in \mathbb{C}\backslash[0,\infty)$, and let

$$f_z = \begin{pmatrix} f_{\mathrm{i},z} \\ f_{\mathrm{e},z} \end{pmatrix} \in H^{3/2}(\Omega_{\mathrm{i}}) \times H^{3/2}(\Omega_{\mathrm{e}}) \tag{4.13}$$

be such that $\gamma_D^{\rm i} f_{{\rm i},z} = \gamma_D^{\rm e} f_{{\rm e},z}$, and

$$-\Delta f_{{\rm i},z} = z f_{{\rm i},z} \text{ and } -\Delta f_{{\rm e},z} = z f_{{\rm e},z}.$$

From the definition of $\mathcal{D}_{\rm i}(z)$ and $\mathcal{D}_{\rm e}(z)$ in (4.3) and (4.4) one concludes that

$$\begin{aligned}\big(\mathcal{D}_{\rm i}(z) + \mathcal{D}_{\rm e}(z)\big)\gamma_D^{\rm i} f_{{\rm i},z} &= \mathcal{D}_{\rm i}(z)\gamma_D^{\rm i} f_{{\rm i},z} + \mathcal{D}_{\rm e}(z)\gamma_D^{\rm e} f_{{\rm e},z} \\ &= \gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}.\end{aligned} \tag{4.14}$$

This also proves that $\mathcal{D}_{\rm i}(z) + \mathcal{D}_{\rm e}(z)$ is injective for $z \in \mathbb{C}\backslash[0,\infty)$. In fact, otherwise there would exist a function $f_z = (f_{{\rm i},z}, f_{{\rm e},z})^\top \neq 0$ as in (4.13) which would satisfy both conditions

$$\gamma_D^{\rm i} f_{{\rm i},z} = \gamma_D^{\rm e} f_{{\rm e},z} \text{ and } \gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z} = 0, \tag{4.15}$$

and hence for all $h \in \operatorname{dom}(H) = H^2(\mathbb{R}^n)$, Green's identity together with the conditions (4.15) would imply

$$\begin{aligned}&(Hh, f_z)_{L^2(\mathbb{R}^n)} - (h, z f_z)_{L^2(\mathbb{R}^n)} \\ &\quad = (-\Delta h_{\rm i}, f_{{\rm i},z})_{L^2(\Omega_{\rm i})} - (h_{\rm i}, -\Delta f_{{\rm i},z})_{L^2(\Omega_{\rm i})} \\ &\qquad\quad + (-\Delta h_{\rm e}, f_{{\rm e},z})_{L^2(\Omega_{\rm e})} - (h_{\rm e}, -\Delta f_{{\rm e},z})_{L^2(\Omega_{\rm e})} \\ &\quad = (\gamma_D^{\rm i} h_{\rm i}, \gamma_N^{\rm i} f_{{\rm i},z})_{L^2(\mathcal{C})} - (\gamma_N^{\rm i} h_{\rm i}, \gamma_D^{\rm i} f_{{\rm i},z})_{L^2(\mathcal{C})} \\ &\qquad\quad + (\gamma_D^{\rm e} h_{\rm e}, \gamma_N^{\rm e} f_{{\rm e},z})_{L^2(\mathcal{C})} - (\gamma_N^{\rm e} h_{\rm e}, \gamma_D^{\rm e} f_{{\rm e},z})_{L^2(\mathcal{C})} \\ &\quad = 0,\end{aligned} \tag{4.16}$$

that is, $f_z \in \operatorname{dom}(H)$ and $Hf_z = zf_z$; a contradiction since $z \in \rho(H)$. Hence,

$$\ker\big(\mathcal{D}_{\rm i}(z) + \mathcal{D}_{\rm e}(z)\big) = \{0\}, \quad z \in \mathbb{C}\backslash[0,\infty),$$

and if we denote the restrictions of $\mathcal{D}_{\rm i}(z)$ and $\mathcal{D}_{\rm e}(z)$ onto $H^{3/2}(\mathcal{C})$ by $\mathcal{D}_{{\rm i},3/2}(z)$ and $\mathcal{D}_{{\rm e},3/2}(z)$, respectively, then also $\ker(\mathcal{D}_{{\rm i},3/2}(z) + \mathcal{D}_{{\rm e},3/2}(z)) = \{0\}$ for $z \in \mathbb{C}\backslash[0,\infty)$. Thus, we have shown that $\mathcal{E}(z)$ and its restriction $\mathcal{E}_{1/2}(z)$ are well-defined for all $z \in \rho(H) = \mathbb{C}\backslash[0,\infty)$.

Furthermore, if the function f_z in (4.13) belongs to $H^2(\Omega_{\rm i}) \times H^2(\Omega_{\rm e})$, that is, $f_z \in \ker(T - zI_{L^2(\mathbb{R}^n)})$, then $\gamma_D^{\rm i} f_{{\rm i},z} = \gamma_D^{\rm e} f_{{\rm e},z} \in H^{3/2}(\mathcal{C})$ and hence besides (4.14) one also has

$$\big(\mathcal{D}_{{\rm i},3/2}(z) + \mathcal{D}_{{\rm e},3/2}(z)\big)\gamma_D^{\rm i} f_{{\rm i},z} = \gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z} \in H^{1/2}(\mathcal{C}). \tag{4.17}$$

One concludes from (4.17) that

$$\mathcal{E}_{1/2}(z)\big(\gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}\big) = \gamma_D^{\rm i} f_{{\rm i},z},$$

and from (4.8) one then obtains

$$\begin{aligned}\big(c\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)\big(\gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}\big) &= c\gamma_D^{\rm i} f_{{\rm i},z} - \big(\gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}\big) \\ &= \Gamma_0 f_z,\end{aligned} \tag{4.18}$$

and

$$\big(\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)\big(\gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}\big) = \alpha\gamma_D^{\rm i} f_{{\rm i},z} - \big(\gamma_N^{\rm i} f_{{\rm i},z} + \gamma_N^{\rm e} f_{{\rm e},z}\big). \tag{4.19}$$

For $z \in \rho(H_{\delta,c}) \cap \rho(H)$ one verifies $\ker(c\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}) = \{0\}$ with the help of (4.18). Then (4.8) and (4.11) yield

$$\operatorname{ran}\big(c\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big) = \operatorname{ran}(\Gamma_0) = H^{1/2}(\mathcal{C}).$$

Thus, it follows from (4.18), (4.19), and (4.9) that

$$\begin{aligned}
&\frac{1}{c-\alpha}\big(\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)\big(c\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)^{-1}\Gamma_0 f_z \\
&\quad = \frac{1}{c-\alpha}\big(\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)\big(\gamma_N^{\mathrm{i}} f_{\mathrm{i},z} + \gamma_N^{\mathrm{e}} f_{\mathrm{e},z}\big) \\
&\quad = \frac{1}{c-\alpha}\Big(\alpha\gamma_D^{\mathrm{i}} f_{\mathrm{i},z} - \big(\gamma_N^{\mathrm{i}} f_{\mathrm{i},z} + \gamma_N^{\mathrm{e}} f_{\mathrm{e},z}\big)\Big) \\
&\quad = \Gamma_1 f_z
\end{aligned}$$

holds for all $z \in \rho(H_{\delta,c}) \cap \rho(H)$. This proves that the Weyl function corresponding to the quasi boundary triple (4.8)–(4.9) is given by (4.12).

Next it will be shown that $M(z)$ and $M(z)^{-1}$ are bounded for $z \in \mathbb{C}\backslash\mathbb{R}$. For this it suffices to check that the operators

$$\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})} \ \text{ and } \ c\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})} \tag{4.20}$$

are bounded and have bounded inverses. The argument is the same for both operators in (4.20) and hence we discuss $\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}$ only. One recalls that

$$\mathcal{D}_{\mathrm{i}}(z) + \mathcal{D}_{\mathrm{e}}(z), \quad z \in \mathbb{C}\backslash\mathbb{R},$$

maps onto $L^2(\mathcal{C})$, is boundedly invertible, and its inverse $\mathcal{E}(z)$ in (4.5) is a compact operator in $L^2(\mathcal{C})$ with $\operatorname{ran}(\mathcal{E}(z)) = H^1(\mathcal{C})$ (see [9, Proposition 3.2 (iii)]). Hence also the restriction $\mathcal{E}_{1/2}(z)$ of $\mathcal{E}(z)$ onto $H^{1/2}(\mathcal{C})$ is bounded in $L^2(\mathcal{C})$. It follows that $\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}$ is bounded, and its closure is given by

$$\overline{\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}} = \alpha\mathcal{E}(z) - I_{L^2(\mathcal{C})} \in \mathcal{L}\big(L^2(\mathcal{C})\big), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.21}$$

In order to show that the inverse $(\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})})^{-1}$ exists and is bounded for $z \in \mathbb{C}\backslash\mathbb{R}$ we first check that

$$\ker\big(\alpha\mathcal{E}(z) - I_{L^2(\mathcal{C})}\big) = \{0\}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.22}$$

In fact, assume that $z \in \mathbb{C}\backslash\mathbb{R}$ and $\varphi \in L^2(\mathcal{C})$ are such that $\alpha\mathcal{E}(z)\varphi = \varphi$. It follows from $\operatorname{dom}(\mathcal{E}(z)) = \operatorname{ran}(\mathcal{D}_{\mathrm{i}}(z) + \mathcal{D}_{\mathrm{e}}(z)) = L^2(\mathcal{C})$ that there exists $\psi \in H^1(\mathcal{C})$ such that

$$\varphi = \big(\mathcal{D}_{\mathrm{i}}(z) + \mathcal{D}_{\mathrm{e}}(z)\big)\psi, \tag{4.23}$$

and from (4.1)–(4.2) one concludes that there exists a unique

$$f_z = \begin{pmatrix} f_{\mathrm{i},z} \\ f_{\mathrm{e},z} \end{pmatrix} \in H^{3/2}(\Omega_{\mathrm{i}}) \times H^{3/2}(\Omega_{\mathrm{e}})$$

such that

$$\gamma_D^{\mathrm{i}} f_{\mathrm{i},z} = \gamma_D^{\mathrm{e}} f_{\mathrm{e},z} = \psi, \tag{4.24}$$

and

$$-\Delta f_{\mathrm{i},z} = z f_{\mathrm{i},z} \ \text{ and } \ -\Delta f_{\mathrm{e},z} = z f_{\mathrm{e},z}.$$

Since $\varphi = \alpha\mathcal{E}(z)\varphi = \alpha\psi$ by (4.23), one obtains from (4.14), (4.24), and (4.23) that

$$\begin{aligned}\gamma_N^{\mathrm{i}} f_{\mathrm{i},z} + \gamma_N^{\mathrm{e}} f_{\mathrm{e},z} &= \big(\mathcal{D}_{\mathrm{i}}(z) + \mathcal{D}_{\mathrm{e}}(z)\big)\gamma_D^{\mathrm{i}} f_{\mathrm{i},z} \\ &= \big(\mathcal{D}_{\mathrm{i}}(z) + \mathcal{D}_{\mathrm{e}}(z)\big)\psi \\ &= \varphi \\ &= \alpha\psi \\ &= \alpha\gamma_D^{\mathrm{i}} f_{\mathrm{i},z}.\end{aligned} \tag{4.25}$$

For $h = (h_{\mathrm{i}}, h_{\mathrm{e}})^\top \in \mathrm{dom}(H_{\delta,\alpha})$ one has

$$\gamma_D^{\mathrm{i}} h_{\mathrm{i}} = \gamma_D^{\mathrm{e}} h_{\mathrm{e}} \;\text{ and }\; \gamma_N^{\mathrm{i}} h_{\mathrm{i}} + \gamma_N^{\mathrm{e}} h_{\mathrm{e}} = \alpha\gamma_D^{\mathrm{i}} h_{\mathrm{i}}, \tag{4.26}$$

and in a similar way as in (4.16), Green's identity together with (4.24), (4.25), and (4.26) imply

$$\begin{aligned}&(H_{\delta,\alpha} h, f_z)_{L^2(\mathbb{R}^n)} - (h, z f_z)_{L^2(\mathbb{R}^n)} \\ &\quad = (-\Delta h_{\mathrm{i}}, f_{\mathrm{i},z})_{L^2(\Omega_{\mathrm{i}})} - (h_{\mathrm{i}}, -\Delta f_{\mathrm{i},z})_{L^2(\Omega_{\mathrm{i}})} \\ &\qquad + (-\Delta h_{\mathrm{e}}, f_{\mathrm{e},z})_{L^2(\Omega_{\mathrm{e}})} - (h_{\mathrm{e}}, -\Delta f_{\mathrm{e},z})_{L^2(\Omega_{\mathrm{e}})} \\ &\quad = (\gamma_D^{\mathrm{i}} h_{\mathrm{i}}, \gamma_N^{\mathrm{i}} f_{\mathrm{i},z})_{L^2(\mathcal{C})} - (\gamma_N^{\mathrm{i}} h_{\mathrm{i}}, \gamma_D^{\mathrm{i}} f_{\mathrm{i},z})_{L^2(\mathcal{C})} \\ &\qquad + (\gamma_D^{\mathrm{e}} h_{\mathrm{e}}, \gamma_N^{\mathrm{e}} f_{\mathrm{e},z})_{L^2(\mathcal{C})} - (\gamma_N^{\mathrm{e}} h_{\mathrm{e}}, \gamma_D^{\mathrm{e}} f_{\mathrm{e},z})_{L^2(\mathcal{C})} \\ &\quad = \big(\gamma_D^{\mathrm{i}} h_{\mathrm{i}}, \gamma_N^{\mathrm{i}} f_{\mathrm{i},z} + \gamma_N^{\mathrm{e}} f_{\mathrm{e},z}\big)_{L^2(\mathcal{C})} - \big(\gamma_N^{\mathrm{i}} h_{\mathrm{i}} + \gamma_N^{\mathrm{e}} h_{\mathrm{e}}, \gamma_D^{\mathrm{i}} f_{\mathrm{i},z}\big)_{L^2(\mathcal{C})} \\ &\quad = \big(\gamma_D^{\mathrm{i}} h_{\mathrm{i}}, \alpha\gamma_D^{\mathrm{i}} f_{\mathrm{i},z}\big)_{L^2(\mathcal{C})} - \big(\alpha\gamma_D^{\mathrm{i}} h_{\mathrm{i}}, \gamma_D^{\mathrm{i}} f_{\mathrm{i},z}\big)_{L^2(\mathcal{C})} \\ &\quad = 0.\end{aligned}$$

As $H_{\delta,\alpha}$ is self-adjoint one concludes that $f_z \in \mathrm{dom}(H_{\delta,\alpha})$ and

$$f_z \in \ker(H_{\delta,\alpha} - z I_{L^2(\mathbb{R}^n)}).$$

Since $z \in \mathbb{C}\backslash\mathbb{R}$, this yields $f_z = 0$ and therefore, $\psi = \gamma_D^{\mathrm{i}} f_{\mathrm{i},z} = 0$ and hence $\varphi = 0$ by (4.23), implying (4.22).

Since $\mathcal{E}(z)$ is a compact operator in $L^2(\mathcal{C})$ (see [9, Proposition 3.2 (*iii*)]) also $\alpha\mathcal{E}(z)$ is compact and together with (4.22) one concludes that

$$(\alpha\mathcal{E}(z) - I_{L^2(\mathcal{C})})^{-1} \in \mathcal{L}\big(L^2(\mathcal{C})\big). \tag{4.27}$$

Hence also the restriction

$$\big(\alpha\mathcal{E}_{1/2}(z) - I_{L^2(\mathcal{C})}\big)^{-1}$$

is a bounded operator in $L^2(\mathcal{C})$. Summing up, we have shown that the operators in (4.20) are bounded and have bounded inverses for all $z \in \mathbb{C}\backslash\mathbb{R}$, and hence the values $M(z)$ of the Weyl function in (4.12) are bounded and have bounded inverses for all $z \in \mathbb{C}\backslash\mathbb{R}$. From (4.12), (4.21) and (4.27) it follows that that the closures of the operators $M(z)$, $z \in \mathbb{C}\backslash\mathbb{R}$, in $L^2(\mathcal{C})$ are given by the operators $\mathcal{M}_\alpha(z)$ in (4.6), (4.7).

Step 3. Now we check that the operators $\{H_{\delta,c}, H_{\delta,\alpha}\}$ and the Weyl function corresponding to the quasi boundary triple $\{L^2(\mathcal{C}), \Gamma_0, \Gamma_1\}$ in Step 1 satisfy the assumptions of Theorem 3.1 for $n \in \mathbb{N}$, $n \geq 2$, and all $k \geq (n-3)/4$.

In fact, the sign condition (3.4) follows from the assumption $\alpha(x) < c$ and the fact that the closed quadratic forms $\mathfrak{h}_{\delta,\alpha}$ and $\mathfrak{h}_{\delta,c}$ associated to $H_{\delta,\alpha}$ and $H_{\delta,c}$ satisfy the inequality $\mathfrak{h}_{\delta,c} \leq \mathfrak{h}_{\delta,\alpha}$. More precisely, the inequality for the quadratic forms yields $\inf(\sigma(H_{\delta,c})) \leq \inf(\sigma(H_{\delta,\alpha}))$, and for $\zeta < \inf(\sigma(H_{\delta,c}))$ the forms $\mathfrak{h}_{\delta,c} - \zeta$ and $\mathfrak{h}_{\delta,\alpha} - \zeta$ are both nonnegative, satisfy the inequality $\mathfrak{h}_{\delta,c} - \zeta \leq \mathfrak{h}_{\delta,\alpha} - \zeta$, and hence the resolvents of the corresponding nonnegative self-adjoint operators $H_{\delta,c} - \zeta I_{L^2(\mathbb{R}^n)}$ and $H_{\delta,\alpha} - \zeta I_{L^2(\mathbb{R}^n)}$ satisfy the inequality

$$(H_{\delta,c} - \zeta I_{L^2(\mathbb{R}^n)})^{-1} \geq (H_{\delta,\alpha} - \zeta I_{L^2(\mathbb{R}^n)})^{-1}, \quad \zeta < \inf(\sigma(H_{\delta,c}))$$

(see, e.g., [30, Chapter VI, § 2.6] or [15, Chapter 10, §2, Theorem 6]). Thus the sign condition (3.4) in the assumptions of Theorem 3.1 holds.

In order to verify the $\mathfrak{S}_p$-conditions

$$\overline{\gamma(z)}^{(p)} \big(M(z)^{-1}\gamma(\overline{z})^*\big)^{(q)} \in \mathfrak{S}_1\big(L^2(\mathbb{R}^n)\big), \quad p+q = 2k, \tag{4.28}$$

$$\big(M(z)^{-1}\gamma(\overline{z})^*\big)^{(q)} \overline{\gamma(z)}^{(p)} \in \mathfrak{S}_1\big(L^2(\mathcal{C})\big), \quad p+q = 2k, \tag{4.29}$$

and

$$\frac{d^j}{dz^j}\overline{M(z)} \in \mathfrak{S}_{(2k+1)/j}\big(L^2(\mathcal{C})\big), \quad j = 1, \dots, 2k+1, \tag{4.30}$$

for all $z \in \rho(H_{\delta,c}) \cap \rho(H_{\delta,\alpha})$ in the assumptions of Theorem 3.1, one first recalls the smoothing property

$$(H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-1} f \in H^{k+2}(\Omega_{\rm i}) \times H^{k+2}(\Omega_{\rm e}) \tag{4.31}$$

for $f \in H^k(\Omega_{\rm i}) \times H^k(\Omega_{\rm e})$ and $k \in \mathbb{N}_0$, which follows, for instance, from [36, Theorem 4.20]. Next one observes that (2.1), (4.9), and the definition of $H_{\delta,c}$ imply

$$\begin{aligned}
\gamma(\overline{z})^* f &= \Gamma_1 (H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-1} f \\
&= (c-\alpha)^{-1}\big(\alpha\gamma_D^{\rm i} - (\gamma_N^{\rm i} + \gamma_N^{\rm e})\big)(H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-1} f \\
&= (c-\alpha)^{-1}\big(c\gamma_D^{\rm i} - (\gamma_N^{\rm i} + \gamma_N^{\rm e}) + (\alpha - c)\gamma_D^{\rm i}\big)(H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-1} f,
\end{aligned}$$

which yields

$$\gamma(\overline{z})^* f = -\gamma_D^{\rm i} (H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-1} f, \quad f \in L^2(\mathbb{R}^n). \tag{4.32}$$

Hence (2.2), (4.31), and Lemma 4.2 imply

$$\big(\gamma(\overline{z})^*\big)^{(q)} = -q!\,\gamma_D^{\rm i} (H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-(q+1)} \in \mathfrak{S}_r\big(L^2(\mathbb{R}^n), L^2(\mathcal{C})\big) \tag{4.33}$$

for $r > (n-1)/[2q + (3/2)]$, $z \in \rho(H_{\delta,c})$ and $q \in \mathbb{N}_0$ (cf. [12, Lemma 3.1] for the case $c = 0$). One also has

$$\overline{\gamma(z)}^{(p)} \in \mathfrak{S}_r\big(L^2(\mathcal{C}), L^2(\mathbb{R}^n)\big), \quad r > (n-1)/[2p + (3/2)], \tag{4.34}$$

for all $z \in \rho(H_{\delta,c})$ and $p \in \mathbb{N}_0$. Furthermore,

$$\frac{d^j}{dz^j}\overline{M(z)} = j!\,\gamma(\overline{z})^* (H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-(j-1)}\overline{\gamma(z)} \tag{4.35}$$

by (2.3) and with the help of (4.32) it follows that

$$\gamma(\overline{z})^*(H_{\delta,c}-zI_{L^2(\mathbb{R}^n)})^{-(j-1)} = -\gamma_D^{\mathrm{i}}(H_{\delta,c}-zI_{L^2(\mathbb{R}^n)})^{-j} \in \mathfrak{S}_x\big(L^2(\mathbb{R}^n),L^2(\mathcal{C})\big)$$

for $x>(n-1)/[2j-(1/2)]$. Moreover, we have $\overline{\gamma(z)}\in\mathfrak{S}_y(L^2(\mathcal{C}),L^2(\mathbb{R}^n))$ for $y>2(n-1)/3$ by (4.34) and hence it follows from (4.35) and the well-known property $PQ\in\mathfrak{S}_w$ for $P\in\mathfrak{S}_x$, $Q\in\mathfrak{S}_y$, and $x^{-1}+y^{-1}=w^{-1}$, that

$$\frac{d^j}{dz^j}\overline{M(z)}\in\mathfrak{S}_w\big(L^2(\mathcal{C})\big), \quad w>(n-1)/(2j+1),\ z\in\rho(H_{\delta,c}),\ j\in\mathbb{N}. \tag{4.36}$$

One observes that

$$\frac{d}{dz}\big[\overline{M(z)}\big]^{-1} = -\big[\overline{M(z)}\big]^{-1}\bigg(\frac{d}{dz}\overline{M(z)}\bigg)\big[\overline{M(z)}\big]^{-1}, \quad z\in\rho(H_{\delta,c})\cap\rho(H_{\delta,\alpha}),$$

that $\big[\overline{M(z)}\big]^{-1}$ is bounded, and by (4.36) that for $j\in\mathbb{N}$ also

$$\frac{d^j}{dz^j}\big[\overline{M(z)}\big]^{-1}\in\mathfrak{S}_w\big(L^2(\mathcal{C})\big), \quad w>(n-1)/(2j+1),\ z\in\rho(H_{\delta,c})\cap\rho(H_{\delta,\alpha}); \tag{4.37}$$

we leave the formal induction step to the reader. Therefore,

$$\begin{aligned}
\big(M(z)^{-1}\gamma(\overline{z})^*\big)^{(q)} &= \Big(\big[\overline{M(z)}\big]^{-1}\gamma(\overline{z})^*\Big)^{(q)}\\
&= \sum_{\substack{p+m=q\\ p,m\geqslant 0}}\binom{q}{p}\Big(\big[\overline{M(z)}\big]^{-1}\Big)^{(p)}\big(\gamma(\overline{z})^*\big)^{(m)}\\
&= \big[\overline{M(z)}\big]^{-1}\big(\gamma(\overline{z})^*\big)^{(q)} + \sum_{\substack{p+m=q\\ p>0,m\geq 0}}\binom{q}{p}\Big(\big[\overline{M(z)}\big]^{-1}\Big)^{(p)}\big(\gamma(\overline{z})^*\big)^{(m)},
\end{aligned} \tag{4.38}$$

and one has

$$\big[\overline{M(z)}\big]^{-1}(\gamma(\overline{z})^*)^{(q)}\in\mathfrak{S}_r\big(L^2(\mathbb{R}^n),L^2(\mathcal{C})\big)$$

for $r>(n-1)/[2q+(3/2)]$ by (4.33) and each summand (and hence also the finite sum) on the right-hand side in (4.38) is in $\mathfrak{S}_r(L^2(\mathbb{R}^n),L^2(\mathcal{C}))$ for $r>(n-1)/[2p+1+2m+(3/2)]=(n-1)/[2q+(5/2)]$, which follows from (4.37) and (4.33). Hence one has

$$\big(M(z)^{-1}\gamma(\overline{z})^*\big)^{(q)}\in\mathfrak{S}_r\big(L^2(\mathbb{R}^n),L^2(\mathcal{C})\big) \tag{4.39}$$

for $r>(n-1)/[2q+(3/2)]$ and $z\in\rho(H_{\delta,c})\cap\rho(H_{\delta,\alpha})$. From (4.34) and (4.39) one then concludes

$$\overline{\gamma(z)}^{(p)}\big(M(z)^{-1}\gamma(\overline{z})^*\big)^{(q)}\in\mathfrak{S}_r\big(L^2(\mathbb{R}^n)\big)$$

for $r>(n-1)/[2(p+q)+3]=(n-1)/(4k+3)$, and since $k\geq(n-3)/4$, one has $1>(n-1)/(4k+3)$, that is, the trace class condition (4.28) is satisfied. The same argument shows that (4.29) is satisfied. Finally, (4.30) follows from (4.36) and the fact that $k\geq(n-3)/4$ implies

$$\frac{2k+1}{j}\geq\frac{n-1}{2j}>\frac{n-1}{2j+1}, \quad j=1,\dots,2k+1.$$

Hence the assumptions in Theorem 3.1 are satisfied with S in Step 1, the quasi boundary triple in (4.8)–(4.9), the corresponding γ-field, and Weyl function in (4.12). Hence, Theorem 3.1 yields assertion (i) in Theorem 4.3 with H replaced by $H_{\delta,c}$. In addition, for any orthonormal basis $\{\varphi_j\}_{j\in J}$ in $L^2(\mathcal{C})$, the function

$$\xi_\alpha(\lambda) = \sum_{j\in J} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\big(\mathrm{Im}\big(\log(\mathcal{M}_\alpha(\lambda+i\varepsilon))\big)\varphi_j,\varphi_j\big)_{L^2(\mathcal{C})} \text{ for a.e. } \lambda\in\mathbb{R}$$

is a spectral shift function for the pair $(H_{\delta,c}, H_{\delta,\alpha})$ such that $\xi_\alpha(\lambda)=0$ for $\lambda < \inf(\sigma(H_{\delta,c})) \leq \inf(\sigma(H_{\delta,\alpha}))$ and the trace formula

$$\begin{aligned}
&\mathrm{tr}_{L^2(\mathbb{R}^n)}\big((H_{\delta,\alpha} - zI_{L^2(\mathbb{R}^n)})^{-(2k+1)} - (H_{\delta,c} - zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big)\\
&\quad = -(2k+1)\int_{\mathbb{R}} \frac{\xi_\alpha(\lambda)\,d\lambda}{(\lambda-z)^{2k+2}}, \quad z\in\rho(H_{\delta,c})\cap\rho(H_{\delta,\alpha}),
\end{aligned}$$

holds.

The above considerations remain valid in the special case $\alpha=0$ which corresponds to the pair $(H_{\delta,c}, H)$ and yields an analogous representation for a spectral shift function ξ_0. Finally it follows from the considerations in the end of Section 3 (see (3.5)) that

$$\begin{aligned}
\xi(\lambda) &= \xi_\alpha(\lambda) - \xi_0(\lambda)\\
&= \sum_{j\in J}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\Big(\big(\mathrm{Im}\big(\log(\mathcal{M}_\alpha(\lambda+i\varepsilon)) - \log(\mathcal{M}_0(\lambda+i\varepsilon))\big)\big)\varphi_j,\varphi_j\Big)_{L^2(\mathcal{C})}
\end{aligned}$$

for a.e. $\lambda\in\mathbb{R}$ is a spectral shift function for the pair $(H, H_{\delta,\alpha})$ such that $\xi(\lambda) = 0$ for $\lambda < \inf(\sigma(H_{\delta,c})) \leq \inf\{\sigma(H),\sigma(H_{\delta,\alpha})\}$. This completes the proof of Theorem 4.3. □

In space dimensions $n=2$ and $n=3$ one can choose $k=0$ in Theorem 4.3 and together with Corollary 3.2 one obtains the following result.

Corollary 4.4. *Let the assumptions and $\mathcal{M}_\alpha$ and $\mathcal{M}_0$ be as in Theorem 4.3, and suppose that $n=2$ or $n=3$. Then the following assertions (i)–(iii) hold:*

(i) *The difference of the resolvents of H and $H_{\delta,\alpha}$ is a trace class operator, that is, for all $z\in\rho(H_{\delta,\alpha}) = \rho(H)\cap\rho(H_{\delta,\alpha})$,*

$$\big[(H_{\delta,\alpha} - zI_{L^2(\mathbb{R}^n)})^{-1} - (H - zI_{L^2(\mathbb{R}^n)})^{-1}\big] \in \mathfrak{S}_1\big(L^2(\mathbb{R}^n)\big).$$

(ii) $\mathrm{Im}(\log(\mathcal{M}_\alpha(z))) \in \mathfrak{S}_1(L^2(\mathcal{C}))$ *and* $\mathrm{Im}(\log(\mathcal{M}_0(z))) \in \mathfrak{S}_1(L^2(\mathcal{C}))$ *for all $z\in\mathbb{C}\backslash\mathbb{R}$, and the limits*

$$\mathrm{Im}\big(\log(\mathcal{M}_\alpha(\lambda+i0))\big) := \lim_{\varepsilon\downarrow 0}\mathrm{Im}\big(\log(\mathcal{M}_\alpha(\lambda+i\varepsilon))\big)$$

and

$$\mathrm{Im}\big(\log(\mathcal{M}_0(\lambda+i0))\big) := \lim_{\varepsilon\downarrow 0}\mathrm{Im}\big(\log(\mathcal{M}_0(\lambda+i\varepsilon))\big)$$

exist for a.e. $\lambda\in\mathbb{R}$ in $\mathfrak{S}_1(L^2(\mathcal{C}))$.

(*iii*) *The function defined by*

$$\xi(\lambda) = \frac{1}{\pi}\,\mathrm{tr}_{L^2(\mathcal{C})}\big(\mathrm{Im}\,\big(\log(\mathcal{M}_\alpha(\lambda+i0)) - \log(\mathcal{M}_0(\lambda+i0))\big)\big)$$

for a.e. $\lambda\in\mathbb{R}$ *is a spectral shift function for the pair* $(H, H_{\delta,\alpha})$ *such that* $\xi(\lambda)=0$ *for* $\lambda<\inf(\sigma(H_{\delta,c}))$ *and the trace formula*

$$\mathrm{tr}_{L^2(\mathbb{R}^n)}\big((H_{\delta,\alpha}-zI_{L^2(\mathbb{R}^n)})^{-1} - (H-zI_{L^2(\mathbb{R}^n)})^{-1}\big) = -\int_{\mathbb{R}} \frac{\xi(\lambda)\,d\lambda}{(\lambda-z)^2}$$

is valid for all $z\in\rho(H_{\delta,\alpha})=\rho(H)\cap\rho(H_{\delta,\alpha})$.

In the special case $\alpha<0$, Theorem 4.3 simplifies slightly since in that case the sign condition (3.4) in Theorem 3.1 is satisfied by the pair $(H, H_{\delta,\alpha})$. Hence it is not necessary to introduce the operator $H_{\delta,c}$ as a comparison operator in the proof of Theorem 4.3. Instead, one considers the operators S and T in Step 1 of the proof of Theorem 4.3, and defines the boundary maps by

$$\Gamma_0 f = -\gamma_N^{\mathrm{i}} f_{\mathrm{i}} - \gamma_N^{\mathrm{e}} f_{\mathrm{e}}, \quad \mathrm{dom}(\Gamma_0)=\mathrm{dom}(T),$$

and

$$\Gamma_1 f = -\gamma_D^{\mathrm{i}} f_{\mathrm{i}} + \frac{1}{\alpha}\big(\gamma_N^{\mathrm{i}} f_{\mathrm{i}} + \gamma_N^{\mathrm{e}} f_{\mathrm{e}}\big), \quad \mathrm{dom}(\Gamma_1)=\mathrm{dom}(T).$$

In this case the corresponding Weyl function is given by

$$M(z) = \mathcal{E}_{1/2}(z) - \alpha^{-1} I_{L^2(\mathcal{C})}, \quad z\in\mathbb{C}\backslash\mathbb{R},$$

and hence the next statement follows in the same way as Theorem 4.3 from our abstract result Theorem 3.1.

Theorem 4.5. *Assume Hypothesis* 4.1, *let* $\mathcal{E}(z)$ *be defined as in* (4.5), *and let* $\alpha\in C^1(\mathcal{C})$ *be a real-valued function such that* $\alpha(x)<0$ *for all* $x\in\mathcal{C}$. *Then the following assertions* (*i*) *and* (*ii*) *hold for* $k\in\mathbb{N}_0$ *such that* $k\geq(n-3)/4$:

(*i*) *The difference of the* $(2k+1)$*-th power of the resolvents of* H *and* $H_{\delta,\alpha}$ *is a trace class operator, that is,*

$$\big[(H_{\delta,\alpha}-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)} - (H-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big] \in \mathfrak{S}_1\big(L^2(\mathbb{R}^n)\big)$$

holds for all $z\in\rho(H_{\delta,\alpha})=\rho(H)\cap\rho(H_{\delta,\alpha})$.

(*ii*) *For any orthonormal basis* $(\varphi_j)_{j\in J}$ *in* $L^2(\mathcal{C})$ *the function defined by*

$$\xi(\lambda) = \sum_{j\in J}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\big(\mathrm{Im}\big(\log(\mathcal{E}(t+i\varepsilon) - \alpha^{-1}I_{L^2(\mathcal{C})})\big)\varphi_j,\varphi_j\big)_{L^2(\mathcal{C})}$$

for a.e. $\lambda\in\mathbb{R}$ *is a spectral shift function for the pair* $(H, H_{\delta,\alpha})$ *such that* $\xi(\lambda)=0$ *for* $\lambda<0$ *and the trace formula*

$$\begin{aligned}\mathrm{tr}_{L^2(\mathbb{R}^n)}\big((H_{\delta,\alpha}-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)} &- (H-zI_{L^2(\mathbb{R}^n)})^{-(2k+1)}\big)\\ &= -(2k+1)\int_{\mathbb{R}}\frac{\xi(\lambda)\,d\lambda}{(\lambda-z)^{2k+2}}\end{aligned}$$

is valid for all $z\in\mathbb{C}\backslash[0,\infty)$.

The analog of Corollary 4.4 again holds in the special cases $n = 2$ and $n = 3$; we omit further details.

Acknowledgments. J.B. is most grateful for the stimulating research stay and the hospitality at the Graduate School of Mathematical Sciences of the University of Tokyo from April to July 2016, where parts of this paper were written. F.G. is indebted to all organizers of the IWOTA 2017 Conference for creating such a stimulating atmosphere and for the great hospitality in Chemnitz, Germany, August 14–18. The authors also wish to thank Hagen Neidhardt for fruitful discussions and helpful remarks. Finally, we thank the anonymous referee and Albrecht Böttcher for a careful reading of our manuscript and for very helpful comments.

This work is supported by International Relations and Mobility Programs of the TU Graz and the Austrian Science Fund (FWF), project P 25162-N26.

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