



# Spectral Theory for Schrödinger Operators with $\delta$ -Interactions Supported on Curves in $\mathbb{R}^3$

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**Abstract.** The main objective of this paper is to systematically develop a spectral and scattering theory for self-adjoint Schrödinger operators with  $\delta$ -interactions supported on closed curves in  $\mathbb{R}^3$ . We provide bounds for the number of negative eigenvalues depending on the geometry of the curve, prove an isoperimetric inequality for the principal eigenvalue, derive Schatten–von Neumann properties for the resolvent difference with the free Laplacian, and establish an explicit representation for the scattering matrix.

## 1. Introduction

Schrödinger operators with singular interactions supported on sets of Lebesgue measure zero were suggested in the physics literature as solvable models in quantum mechanics in [11, 37, 45, 48, 60]. They appear, e.g., in the modeling of zero-range interactions of quantum particles [21, 22, 51, 52], in the theory of photonic crystals [41], and in quantum few-body systems in strong magnetic fields [19]. The mathematical investigation of their spectral and scattering properties attracted a lot of attention during the last decades. First studies were mostly devoted to singular interactions supported on a discrete set of points, see the monograph [4] and [34, Chapter 5]. Later on, singular interactions supported on more general curves, surfaces, and manifolds gained much attention; there is an extensive literature on Schrödinger operators with  $\delta$ -interactions supported on manifolds of codimension one, see, e.g. [5, 9, 15, 17, 26, 29, 34–36] and the references therein. Manifolds of higher codimension were first treated in [16] in the very special case of an interaction supported on a straight line in  $\mathbb{R}^3$ . More general curves were considered in [12, 18, 27, 30–33, 44, 46, 47, 53, 57, 59].

In the present paper, we systematically develop a spectral and scattering theory for Schrödinger operators with singular interactions supported on curves in the three-dimensional space. More specifically, for a compact, closed, regular  $C^2$ -curve  $\Sigma \subset \mathbb{R}^3$  we consider the self-adjoint Schrödinger operator  $-\Delta_{\Sigma,\alpha}$  in  $L^2(\mathbb{R}^3)$ , which corresponds to the formal differential expression

$$-\Delta - \frac{1}{\alpha}\delta(\cdot - \Sigma), \tag{1.1}$$

where  $\alpha \in \mathbb{R} \setminus \{0\}$  is the inverse strength of interaction. The mathematically rigorous definition of  $-\Delta_{\Sigma,\alpha}$  is more involved than in the case of, e.g., a curve in  $\mathbb{R}^2$  or a hypersurface in  $\mathbb{R}^3$ . For our purposes, an explicit characterization of the domain and action of  $-\Delta_{\Sigma,\alpha}$  is essential; here the key difficulty is to define an appropriate generalized trace map for functions which are not sufficiently regular; see Sect. 2 for the details. Our method is strongly inspired by [57] and the abstract concept of boundary triples [7, 8, 20, 23, 24], and can also be viewed as a special case of the more general approach in [53] (see Example 3.5 therein); cf. [18, 30, 33, 59] for equivalent alternative definitions.

The main results of this paper deal with spectral and scattering properties of  $-\Delta_{\Sigma,\alpha}$  and extend and complement results in [18, 25, 27, 28, 31, 44, 57]. First, we verify that the operator  $-\Delta_{\Sigma,\alpha}$  is in fact self-adjoint; along with this, in Theorem 3.1 we establish a Krein-type formula for the resolvent difference of  $-\Delta_{\Sigma,\alpha}$  and the free Laplacian  $-\Delta_{\text{free}}$ . Using this formula, we show that the resolvent difference

$$(-\Delta_{\Sigma,\alpha} - \lambda)^{-1} - (-\Delta_{\text{free}} - \lambda)^{-1}, \quad \lambda \in \rho(-\Delta_{\Sigma,\alpha}) \cap \rho(-\Delta_{\text{free}}), \tag{1.2}$$

is compact; in particular, the essential spectrum of  $-\Delta_{\Sigma,\alpha}$  equals  $[0, \infty)$ . Moreover, we provide a Birman–Schwinger principle for the negative eigenvalues of  $-\Delta_{\Sigma,\alpha}$  and employ this principle for a more detailed study of these eigenvalues. In fact, in Theorem 3.3 we show that the negative spectrum is always finite and we prove upper and lower estimates for the number of negative eigenvalues, depending on the (inverse) strength of interaction  $\alpha$  and the geometry of the curve; these results complement the estimates in [18, 31, 43, 44]. In the case that  $\Sigma$  is a circle, our estimates lead to an explicit formula for the number of negative eigenvalues. As a further main result, in Theorem 3.6 we prove that amongst all curves of a fixed length the principle eigenvalue of  $-\Delta_{\Sigma,\alpha}$  is maximized by the circle. With this result we give an affirmative answer to an open problem formulated in [26, Section 7.8]. Our proof is inspired by related considerations for  $\delta$ -interactions supported on loops in the plane in [25, 28].

Another group of results focuses on a more detailed comparison of  $-\Delta_{\Sigma,\alpha}$  with the free Laplacian. From a careful analysis of the operators involved in the Krein-type resolvent formula, we obtain an asymptotic upper bound for the singular values  $s_1(\lambda) \geq s_2(\lambda) \geq \dots$  of the resolvent difference (1.2) in Theorem 3.2,

$$s_k(\lambda) = O\left(\frac{1}{k^2 \ln k}\right) \quad \text{as } k \rightarrow +\infty. \tag{1.3}$$

In particular, the resolvent difference in (1.2) belongs to the Schatten–von Neumann class  $\mathfrak{S}_p$  for any  $p > 1/2$ ; this improves the trace class estimate in [18] and is in accordance with a previous observation in a periodic setting in [27, Remark 4.1]. Note that, as a consequence of (1.3), the absolutely continuous spectrum of  $-\Delta_{\Sigma,\alpha}$  equals  $[0, \infty)$  and the wave operators for the scattering pair  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma,\alpha}\}$  exist and are complete. In Theorem 3.8, a representation of the associated scattering matrix is given in terms of an explicit operator function which acts in  $L^2(\Sigma)$ ; this complements earlier investigations in [18, Section 3]. Its proof relies on an abstract approach developed recently in [10].

The paper is organized as follows. In Sect. 2, we discuss in detail the mathematically rigorous definition of the operator  $-\Delta_{\Sigma,\alpha}$ . Section 3 contains all main results of this paper. Their proofs are carried out in the remainder of this paper. In fact, Sect. 4 is preparatory and contains the analysis of the Birman–Schwinger operator. The actual proofs of Theorems 3.1–3.8 are contained in Sect. 5. In a short appendix, the notions of quasi boundary triples and their Weyl functions from extension theory of symmetric operators are reviewed and it is shown how the operators  $-\Delta_{\text{free}}$  and  $-\Delta_{\Sigma,\alpha}$  fit into this abstract scheme.

## 2. Definition of the Operator $-\Delta_{\Sigma,\alpha}$

In this section, we define the operator  $-\Delta_{\Sigma,\alpha}$  associated with the differential expression (1.1) in  $L^2(\mathbb{R}^3)$ . On a formal level, we interpret the action of (1.1) as

$$\mathcal{A}_\alpha u := -\Delta u - \frac{1}{\alpha} u|_\Sigma \cdot \delta_\Sigma. \tag{2.1}$$

It will be shown that  $\mathcal{A}_\alpha$  gives rise to a self-adjoint operator in  $L^2(\mathbb{R}^3)$ . The key difficulty in the definition of this operator is to specify a suitable domain. Note that the Sobolev space  $H^2(\mathbb{R}^3)$  is not a suitable domain as  $u|_\Sigma \cdot \delta_\Sigma \notin L^2(\mathbb{R}^3)$  for all those  $u \in H^2(\mathbb{R}^3)$  which do not vanish identically on  $\Sigma$ . On the other hand, any proper subspace of  $H^2(\mathbb{R}^3)$  will turn out to be too small for  $-\Delta_{\Sigma,\alpha}$  to become self-adjoint in  $L^2(\mathbb{R}^3)$ . Thus, it is necessary to include suitable more singular elements in the domain of the operator. This requires the definition of a generalized trace  $u|_\Sigma$  for functions  $u \in L^2(\mathbb{R}^3)$  which are not sufficiently regular.

Let us first fix some notation. We assume that  $\Sigma$  is a compact, closed, regular  $C^2$ -curve in  $\mathbb{R}^3$  of finite length  $L > 0$  without self-intersections and that  $\sigma : [0, L] \rightarrow \mathbb{R}^3$  is a  $C^2$ -parametrization of  $\Sigma$  with  $|\dot{\sigma}(s)| = 1$  for all  $s \in [0, L]$ . Occasionally, we identify  $\sigma$  with its  $L$ -periodic extension. For  $h \in L^2(\Sigma)$ , we define the distribution  $h\delta_\Sigma$  via

$$\langle h\delta_\Sigma, \varphi \rangle_{-2,2} = \int_\Sigma h(x) \overline{\varphi(x)} d\sigma(x), \quad \varphi \in H^2(\mathbb{R}^3), \tag{2.2}$$

where  $\varphi(x)$  is the evaluation of the continuous function  $\varphi$  at  $x \in \Sigma$ ,  $\langle \cdot, \cdot \rangle_{-2,2}$  denotes the duality between  $H^{-2}(\mathbb{R}^3)$  and  $H^2(\mathbb{R}^3)$ , and  $d\sigma$  denotes integration with respect to the arc length on  $\Sigma$ . It follows from the continuity of the

restriction map  $H^2(\mathbb{R}^3) \ni \varphi \mapsto \varphi|_\Sigma \in L^2(\Sigma)$  (see, e.g., [13, Theorem 24.3]) that  $h\delta_\Sigma \in H^{-2}(\mathbb{R}^3)$  and that  $h \mapsto h\delta_\Sigma$  is a continuous mapping from  $L^2(\Sigma)$  to  $H^{-2}(\mathbb{R}^3)$ . We will often use that  $h\delta_\Sigma \in L^2(\mathbb{R}^3)$  if and only if  $h = 0$ .

For  $\lambda < 0$ , we define the bounded operator

$$\gamma_\lambda : L^2(\Sigma) \rightarrow L^2(\mathbb{R}^3), \quad h \mapsto \gamma_\lambda h = (-\Delta - \lambda)^{-1}(h\delta_\Sigma), \quad (2.3)$$

where  $-\Delta - \lambda$  is viewed as an isomorphism between  $L^2(\mathbb{R}^3)$  and  $H^{-2}(\mathbb{R}^3)$ . In the following lemma, a useful representation of  $\gamma_\lambda$  and the adjoint operator  $\gamma_\lambda^* : L^2(\mathbb{R}^3) \rightarrow L^2(\Sigma)$  is provided. We denote the self-adjoint Laplacian in  $L^2(\mathbb{R}^3)$  with domain  $H^2(\mathbb{R}^3)$  by  $-\Delta_{\text{free}}$ .

**Lemma 2.1.** *Let  $\lambda < 0$ . Then*

$$(\gamma_\lambda h)(x) = \int_\Sigma h(y) \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) \quad (2.4)$$

holds for almost all  $x \in \mathbb{R}^3$  and all  $h \in L^2(\Sigma)$ . Moreover,

$$\gamma_\lambda^* u = ((-\Delta_{\text{free}} - \lambda)^{-1}u)|_\Sigma \quad (2.5)$$

holds for all  $u \in L^2(\mathbb{R}^3)$ .

*Proof.* For  $h \in L^2(\Sigma)$  and  $u \in L^2(\mathbb{R}^3)$ , we have

$$\begin{aligned} \langle \gamma_\lambda h, u \rangle_{L^2(\mathbb{R}^3)} &= \langle \gamma_\lambda h, (-\Delta_{\text{free}} - \lambda)(-\Delta_{\text{free}} - \lambda)^{-1}u \rangle_{L^2(\mathbb{R}^3)} \\ &= \langle (-\Delta - \lambda)(\gamma_\lambda h), (-\Delta - \lambda)^{-1}u \rangle_{-2,2} \\ &= \langle h\delta_\Sigma, (-\Delta - \lambda)^{-1}u \rangle_{-2,2} \\ &= \int_\Sigma h(y) \overline{((-\Delta_{\text{free}} - \lambda)^{-1}u)(y)} d\sigma(y) \\ &= \int_{\mathbb{R}^3} \int_\Sigma h(y) \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) \overline{u(x)} dx, \end{aligned}$$

where we have used (2.2) and the integral representation of  $(-\Delta_{\text{free}} - \lambda)^{-1}$ , see, e.g., [54, (IX.30)]. This proves both (2.4) and (2.5).  $\square$

The identity (2.4) indicates that in general the trace of  $\gamma_\lambda h$  on  $\Sigma$  does not exist due to the singularity of the integral kernel. This motivates the following regularization. Here and in the following, we denote by  $C^{0,1}(\Sigma)$  the space of all complex-valued Lipschitz continuous functions on  $\Sigma$ . Moreover, for  $x = \sigma(s_0) \in \Sigma$  and  $\delta > 0$  let

$$I_\delta^\Sigma(x) = \{\sigma(s) : s \in (s_0 - \delta, s_0 + \delta)\} \quad (2.6)$$

be the open interval in  $\Sigma$  with center  $x$  and length  $2\delta$ . To define the trace of  $\gamma_\lambda h$  in a generalized sense, for  $\lambda \leq 0$ ,  $h \in C^{0,1}(\Sigma)$  and  $x \in \Sigma$ , we set

$$(B_\lambda h)(x) = \lim_{\delta \searrow 0} \left[ \int_{\Sigma \setminus I_\delta^\Sigma(x)} h(y) \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) + h(x) \frac{\ln \delta}{2\pi} \right]; \quad (2.7)$$

due to technical reasons the case  $\lambda = 0$  is included here although  $\gamma_\lambda$  is defined for  $\lambda < 0$  only. It will be shown in Proposition 4.5 that  $B_\lambda$  is a well-defined,

essentially self-adjoint operator in  $L^2(\Sigma)$  for each  $\lambda \leq 0$  and that the domain of its closure  $\overline{B_\lambda}$  is independent of  $\lambda$ . Note that the basic idea in the definition of  $B_\lambda$  is to remove the singularity of  $\gamma_\lambda h$  on  $\Sigma$ . We remark that the limit in the definition of  $B_\lambda$  can also be viewed as the finite part in the sense of Hadamard of the first summand as  $\delta \searrow 0$ ; cf. [49, Chapter 5]. A procedure of this type is frequently employed to define hypersingular integral operators.

With the help of  $B_\lambda$  we can make the following definition.

**Definition 2.2.** Let  $\lambda < 0$ . For  $h \in \text{dom } \overline{B_\lambda}$ , we define the generalized trace  $(\gamma_\lambda h)|_\Sigma$  of  $\gamma_\lambda h$  on  $\Sigma$  by

$$(\gamma_\lambda h)|_\Sigma = \overline{B_\lambda} h \in L^2(\Sigma), \quad h \in \text{dom } \overline{B_\lambda}.$$

Accordingly, for a function  $u = u_c + \gamma_\lambda h$  with  $u_c \in H^2(\mathbb{R}^3)$  and  $h \in \text{dom } \overline{B_\lambda}$  we define its generalized trace  $u|_\Sigma$  on  $\Sigma$  by

$$u|_\Sigma = u_c|_\Sigma + (\gamma_\lambda h)|_\Sigma = u_c|_\Sigma + \overline{B_\lambda} h. \tag{2.8}$$

Note that  $u|_\Sigma$  is well defined. Indeed, the representation of  $u$  as a sum is unique since  $\gamma_\lambda h \in H^2(\mathbb{R}^3)$  implies  $h = 0$ . Moreover, the definition of  $u|_\Sigma$  is independent of the choice of  $\lambda < 0$ ; cf. Sect. 4.3.

Furthermore, note that the expression  $\mathcal{A}_\alpha$  in (2.1) is no longer formal, but makes sense as we have defined the generalized trace  $u|_\Sigma$ . Now we are able to define the Schrödinger operator  $-\Delta_{\Sigma,\alpha}$  corresponding to the differential expression in (1.1) in a rigorous way.

**Definition 2.3.** For  $\alpha \in \mathbb{R} \setminus \{0\}$ , the Schrödinger operator  $-\Delta_{\Sigma,\alpha}$  in  $L^2(\mathbb{R}^3)$  with  $\delta$ -interaction of strength  $\frac{1}{\alpha}$  supported on  $\Sigma$  is defined by

$$-\Delta_{\Sigma,\alpha} u = \mathcal{A}_\alpha u = -\Delta u - \frac{1}{\alpha} u|_\Sigma \cdot \delta_\Sigma,$$

$$\text{dom}(-\Delta_{\Sigma,\alpha}) = \left\{ u = u_c + \gamma_\lambda h : u_c \in H^2(\mathbb{R}^3), h \in \text{dom } \overline{B_\lambda}, \mathcal{A}_\alpha u \in L^2(\mathbb{R}^3) \right\},$$

where  $\lambda < 0$  is arbitrary and the generalized trace  $u|_\Sigma$  is defined in (2.8).

Observe that the operator  $-\Delta_{\Sigma,\alpha}$  is well defined since  $\text{dom } \overline{B_\lambda}$  and the trace  $u|_\Sigma$  do not depend on the choice of  $\lambda$ . Note also that for  $\alpha = +\infty$ , we formally have

$$-\Delta_{\Sigma,+\infty} u = -\Delta u, \quad \text{dom}(-\Delta_{\Sigma,+\infty}) = H^2(\mathbb{R}^3),$$

so that the Schrödinger operator with  $\delta$ -interaction of strength 0 on  $\Sigma$  coincides with the free Laplacian  $-\Delta_{\text{free}}$ ; this will be made precise in Theorem 3.1 (ii) below.

*Remark 2.4.* The definition of  $-\Delta_{\Sigma,\alpha}$  relies on the generalized trace in Definition 2.2 and, thus, on the operator  $B_\lambda$ . As mentioned above, the operator  $B_\lambda$  is designed in such a way that the singularity of  $\gamma_\lambda h$  on  $\Sigma$  is removed; this is done here by the term  $\frac{\ln \delta}{2\pi}$ . However, an alternative choice  $\frac{\ln \delta}{2\pi} + c$  with an arbitrary  $\delta$ -independent constant  $c \in \mathbb{R}$  can be made. This leads to a different operator  $-\Delta_{\Sigma,\alpha}$ , which can be transformed into the operator in Definition 2.3 by adding the same constant  $c$  to  $\alpha$ . For instance, for  $c = -\frac{\ln 2}{2\pi}$  one obtains the family of operators considered in [59].

*Remark 2.5.* For a function  $u = u_c + \gamma_\lambda h \in \text{dom}(-\Delta_{\Sigma,\alpha})$  with  $h \in C^{0,1}(\Sigma)$ , we denote by  $\widehat{u}(s, \delta)$ ,  $s \in [0, L)$ , the mean value of  $u$  over a circle of a sufficiently small radius  $\delta > 0$  centered at  $\sigma(s)$  and being orthogonal to  $\Sigma$  in  $\sigma(s)$ . According to [59, Remark 3] (see also [27, 30]), the functions

$$h_0(s) := 2\pi \lim_{\delta \searrow 0} \frac{\widehat{u}(s, \delta)}{\ln(1/\delta)} \quad \text{and} \quad h_1(s) := \lim_{\delta \searrow 0} \left[ \widehat{u}(s, \delta) - \frac{h_0(s)}{2\pi} \ln \left( \frac{1}{\delta} \right) \right]$$

are well defined and continuous on  $\Sigma$  and the function  $u$  satisfies the following boundary condition

$$h_1(s) = \left( \alpha + \frac{\ln 2}{2\pi} \right) h_0(s).$$

In many-body physics with zero-range interactions, a boundary condition of this type is known as Skorniakov–Ter-Martirosian condition; see [58] and also [21, 50].

### 3. Main Results

In this section, we present all main results of this paper. It will be shown that  $-\Delta_{\Sigma,\alpha}$  is self-adjoint and its spectral and scattering properties will be analyzed. This section is focused on the main statements and does not contain their proofs; these are postponed to Sect. 5 below. In the following, we denote by  $\sigma_p(-\Delta_{\Sigma,\alpha})$ ,  $\sigma_{\text{ess}}(-\Delta_{\Sigma,\alpha})$ , and  $\rho(-\Delta_{\Sigma,\alpha})$  the point spectrum, essential spectrum, and resolvent set of  $-\Delta_{\Sigma,\alpha}$ , respectively.

In the first theorem, we check that  $-\Delta_{\Sigma,\alpha}$  is a self-adjoint operator in  $L^2(\mathbb{R}^3)$ , prove a Birman–Schwinger principle for its negative eigenvalues and compare its resolvent to the resolvent of the free Laplacian  $-\Delta_{\text{free}}$  in a Krein-type formula, which also implies that the difference of the resolvents is compact.

**Theorem 3.1.** *The Schrödinger operator  $-\Delta_{\Sigma,\alpha}$  in Definition 2.3 is self-adjoint in  $L^2(\mathbb{R}^3)$ . Moreover, the following assertions hold.*

- (i) *For each  $\lambda < 0$ , the operator  $\gamma_\lambda$  is an isomorphism between  $\ker(\alpha - \overline{B_\lambda})$  and  $\ker(-\Delta_{\Sigma,\alpha} - \lambda)$ . In particular, for each  $\lambda < 0$*

$$\lambda \in \sigma_p(-\Delta_{\Sigma,\alpha}) \quad \text{if and only if} \quad \alpha \in \sigma_p(\overline{B_\lambda}).$$

- (ii) *The set  $\rho(-\Delta_{\Sigma,\alpha}) \cap (-\infty, 0)$  is nonempty and for each  $\lambda \in \rho(-\Delta_{\Sigma,\alpha}) \cap (-\infty, 0)$ , the resolvent formula*

$$(-\Delta_{\Sigma,\alpha} - \lambda)^{-1} = (-\Delta_{\text{free}} - \lambda)^{-1} + \gamma_\lambda (\alpha - \overline{B_\lambda})^{-1} \gamma_\lambda^* \tag{3.1}$$

*is valid. Furthermore,  $-\Delta_{\Sigma,\alpha}$  converges to  $-\Delta_{\text{free}}$  in the norm resolvent sense as  $\alpha \rightarrow +\infty$ .*

- (iii) *For each  $\lambda \in \rho(-\Delta_{\Sigma,\alpha}) \cap \rho(-\Delta_{\text{free}})$ , the resolvent difference*

$$(-\Delta_{\Sigma,\alpha} - \lambda)^{-1} - (-\Delta_{\text{free}} - \lambda)^{-1} \tag{3.2}$$

*is compact and, in particular,  $\sigma_{\text{ess}}(-\Delta_{\Sigma,\alpha}) = [0, \infty)$ .*

Next, we investigate the resolvent difference of  $-\Delta_{\Sigma,\alpha}$  and the free Laplacian in more detail.

**Theorem 3.2.** *Let  $s_1(\lambda) \geq s_2(\lambda) \geq \dots$  be the singular values of the resolvent difference of  $-\Delta_{\Sigma,\alpha}$  and  $-\Delta_{\text{free}}$  in (3.2), counted with multiplicities. Then*

$$s_k(\lambda) = O\left(\frac{1}{k^2 \ln k}\right) \quad \text{as } k \rightarrow +\infty.$$

*In particular, (3.2) belongs to the Schatten-von Neumann ideal  $\mathfrak{S}_p(L^2(\mathbb{R}^3))$  for each  $p > 1/2$ .*

The logarithmic factor in the estimate for the singular values in the above theorem is related to the fact that the eigenvalues of  $\overline{B_\lambda}$  behave asymptotically as  $-\frac{\ln k}{2\pi}$ , see Proposition 4.5 (iii).

In the following theorem, we show that the discrete spectrum of  $-\Delta_{\Sigma,\alpha}$  is always finite and give estimates for the number  $N_\alpha$  of negative eigenvalues, counted with multiplicities. Let  $R = \frac{L}{2\pi}$  and define the intervals

$$I_{-1} = \left[ \frac{\ln(4R)}{2\pi}, +\infty \right), \quad I_0 = \left[ \frac{\ln(4R)}{2\pi} - \frac{1}{\pi}, \frac{\ln(4R)}{2\pi} \right),$$

and

$$I_r = \left[ \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^{r+1} \frac{1}{2j-1}, \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^r \frac{1}{2j-1} \right), \quad r = 1, 2, \dots,$$

which are disjoint and satisfy  $\mathbb{R} = \bigcup_{r=-1}^\infty I_r$ . Moreover, set

$$d_\Sigma = \int_0^L \int_0^L \left| \frac{1}{4\pi|\sigma(t) - \sigma(s)|} - \frac{1}{4\pi|\tau(t) - \tau(s)|} \right|^2 ds dt \geq 0, \tag{3.3}$$

where  $\sigma$  is the parametrization of  $\Sigma$  fixed in the beginning of Sect. 2 and  $\tau$  denotes an arc length parametrization of a circle of radius  $R$ .

**Theorem 3.3.** *Let  $\alpha \neq 0$  and denote by  $N_\alpha$  the number of negative eigenvalues of  $-\Delta_{\Sigma,\alpha}$ , counted with multiplicities. If  $\alpha - d_\Sigma \geq \frac{\ln(4R)}{2\pi}$  then  $N_\alpha = 0$ . Otherwise,*

$$2r + 1 \leq N_\alpha \leq 2l + 1,$$

*where  $r \geq -1$  and  $l \geq 0$  are such that  $\alpha + d_\Sigma \in I_r$  and  $\alpha - d_\Sigma \in I_l$ . In particular,  $N_\alpha$  is finite and the operator  $-\Delta_{\Sigma,\alpha}$  is bounded from below.*

In the next corollary, the upper and lower bounds on the number  $N_\alpha$  of negative eigenvalues in Theorem 3.3 are made more explicit. This also leads to an asymptotic bound  $N_\alpha = e^{-2\pi\alpha + O(1)}$  as  $\alpha \rightarrow -\infty$ . We mention that a slightly better asymptotic bound was obtained in [31]. For convenience, we make a very small technical restriction and consider the case  $\alpha + d_\Sigma < \frac{\ln(4R)}{2\pi} - \frac{1}{\pi}$  only.

**Corollary 3.4.** *Let  $\alpha \neq 0$  be such that  $\alpha + d_\Sigma < \frac{\ln(4R)}{2\pi} - \frac{1}{\pi}$  and denote by  $N_\alpha$  the number of negative eigenvalues of  $-\Delta_{\Sigma,\alpha}$ , counted with multiplicities. Then the estimate*

$$2Rc^{-1}e^{-2\pi\alpha-\gamma} - 1 - 4(e^{\frac{1}{92}} - 1) < N_\alpha < 2Rce^{-2\pi\alpha-\gamma} + 1 \tag{3.4}$$

*holds, where  $\gamma \approx 0.577216$  is the Euler–Mascheroni constant and  $c := e^{2\pi d_\Sigma}$ . In particular,  $N_\alpha = e^{-2\pi\alpha+O(1)}$  as  $\alpha \rightarrow -\infty$ .*

In the case where  $\Sigma$  is a circle, we have  $d_\Sigma = 0$  and hence from Theorem 3.3 and Corollary 3.4 we immediately obtain the following explicit expressions for the number of negative eigenvalues. For a similar formula in a related context see [44] (cf. also [18]).

**Corollary 3.5.** *Let  $\Sigma$  be a circle of radius  $R$  in  $\mathbb{R}^3$ , let  $\alpha \neq 0$ , and denote by  $N_\alpha$  the number of negative eigenvalues of  $-\Delta_{\Sigma,\alpha}$ , counted with multiplicities. If  $\alpha \geq \frac{\ln(4R)}{2\pi}$ , then  $N_\alpha = 0$ . Otherwise,*

$$N_\alpha = 2r + 1, \quad \text{where } r \geq 0 \text{ is such that } \alpha \in I_r.$$

*If  $\alpha < \frac{\ln(4R)}{2\pi} - \frac{1}{\pi}$ , then the estimate*

$$|N_\alpha - 2Re^{-2\pi\alpha-\gamma}| < 1 + 4(e^{\frac{1}{92}} - 1)$$

*holds.*

Next, we investigate the behavior of the smallest eigenvalue of  $-\Delta_{\Sigma,\alpha}$  when varying  $\Sigma$  among all curves of a given length  $L$ . It turns out that circles are the unique maximizers of the minimum of the spectrum  $\sigma(-\Delta_{\Sigma,\alpha})$  in the case that negative eigenvalues exist. The analog of the following theorem for curves in the two-dimensional space was shown in [25, 28].

**Theorem 3.6.** *Let  $\mathcal{T}$  be a circle in  $\mathbb{R}^3$  of radius  $R = \frac{L}{2\pi}$  and assume that  $\Sigma$  is not a circle. Let  $\alpha < \frac{\ln(4R)}{2\pi}$ . Then*

$$\min \sigma(-\Delta_{\Sigma,\alpha}) < \min \sigma(-\Delta_{\mathcal{T},\alpha}),$$

*where  $-\Delta_{\mathcal{T},\alpha}$  denotes the Schrödinger operator with  $\delta$ -interaction of strength  $\frac{1}{\alpha}$  supported on the circle  $\mathcal{T}$ .*

Finally, we regard the pair  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma,\alpha}\}$  as a scattering system consisting of the unperturbed Laplacian  $-\Delta_{\text{free}}$  and the singularly perturbed operator  $-\Delta_{\Sigma,\alpha}$ . The following corollary is an immediate consequence of Theorem 3.2 and the Birman–Krein theorem [14].

**Corollary 3.7.** *The absolutely continuous spectrum of  $-\Delta_{\Sigma,\alpha}$  is given by*

$$\sigma_{\text{ac}}(-\Delta_{\Sigma,\alpha}) = [0, +\infty).$$

*Moreover, the wave operators for the scattering pair  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma,\alpha}\}$  exist and are complete.*



In the next theorem, we express the scattering matrix of the scattering system  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma, \alpha}\}$  in terms of the limits of a certain explicit operator function, using a result in [10]; we refer to [6, 42, 55, 61] and Appendix A for more details on scattering theory. For our purposes, it is convenient to consider the symmetric operator  $S$  in  $L^2(\mathbb{R}^3)$  defined as

$$Su = -\Delta u, \quad \text{dom } S = \{u \in H^2(\mathbb{R}^3) : u|_{\Sigma} = 0\},$$

which turns out to be the intersection of the self-adjoint operators  $-\Delta_{\text{free}}$  and  $-\Delta_{\Sigma, \alpha}$ . Then  $S$  is a densely defined, closed, symmetric operator with infinite defect numbers. Furthermore, in general  $S$  contains a self-adjoint part which can be split off. More precisely, consider the closed subspace

$$\mathfrak{H}_1 = \overline{\text{span} \bigcup_{\lambda \in \mathbb{C} \setminus [0, \infty)} (\text{ran}(S - \lambda))^\perp}$$

of  $L^2(\mathbb{R}^3)$  and let  $\mathfrak{H}_2 = \mathfrak{H}_1^\perp$ . Then  $S$  admits the orthogonal sum decomposition

$$S = S_1 \oplus S_2$$

with respect to the space decomposition  $L^2(\mathbb{R}^3) = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ , where the closed symmetric operator  $S_1$  is completely non-self-adjoint or simple (cf. [3, Chapter VII]) in  $\mathfrak{H}_1$  and  $S_2$  is a self-adjoint operator in  $\mathfrak{H}_2$  with purely absolutely continuous spectrum. In the following, let  $L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda)$  be a spectral representation of the self-adjoint operator  $S_2$  in  $\mathfrak{H}_2$ ; cf. [6, Chapter 4].

**Theorem 3.8.** *Fix  $\eta < 0$  such that  $0 \in \rho(\overline{B_\eta} - \alpha)$  and define the operator function  $\mathbb{C} \setminus [0, \infty) \ni \lambda \mapsto N(\lambda)$  by*

$$(N(\lambda)h)(x) = \int_{\Sigma} h(y) \frac{e^{i\sqrt{\lambda}|x-y|} - e^{i\sqrt{\eta}|x-y|}}{4\pi|x-y|} d\sigma(y), \tag{3.5}$$

where  $h \in L^2(\Sigma)$  and  $x \in \Sigma$ . Then the following assertions hold.

- (i)  $\text{Im } N(\lambda) \in \mathfrak{S}_1(L^2(\Sigma))$  for all  $\lambda \in \mathbb{C} \setminus [0, \infty)$  and the limit

$$\text{Im } N(\lambda + i0) := \lim_{\varepsilon \searrow 0} \text{Im } N(\lambda + i\varepsilon)$$

exists in  $\mathfrak{S}_1(L^2(\Sigma))$  for a.e.  $\lambda \in [0, \infty)$ .

- (ii) The function  $\lambda \mapsto N(\lambda)$ ,  $\lambda \in \mathbb{C} \setminus [0, \infty)$ , is a Nevanlinna function such that the limit

$$N(\lambda + i0) := \lim_{\varepsilon \searrow 0} N(\lambda + i\varepsilon)$$

exists in the Hilbert–Schmidt norm for a.e.  $\lambda \in [0, \infty)$ . Moreover, for a.e.  $\lambda \in [0, \infty)$  the operator  $N(\lambda + i0) + \overline{B_\eta} - \alpha$  is boundedly invertible.

- (iii) The space  $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$ , where

$$\mathcal{G}_\lambda := \overline{\text{ran}(\text{Im } N(\lambda + i0))} \quad \text{for a.e. } \lambda \in [0, \infty),$$

forms a spectral representation of  $-\Delta_{\text{free}}$ .

(iv) *The scattering matrix  $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$  of the scattering system  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma, \alpha}\}$  acting in the space  $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$  admits the representation*

$$S(\lambda) = \begin{pmatrix} S'(\lambda) & 0 \\ 0 & I_{\mathcal{H}_\lambda} \end{pmatrix}$$

for a.e.  $\lambda \in [0, \infty)$ , where

$$S'(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\text{Im } N(\lambda + i0)} (N(\lambda + i0) + \overline{B_\eta} - \alpha)^{-1} \sqrt{\text{Im } N(\lambda + i0)}.$$

### 4. The Operator $B_\lambda$ and the Generalized Trace

In this section, we discuss properties of the operator  $B_\lambda$  in (2.7) and of the generalized trace defined in (2.8). We verify that the latter is well defined and independent of  $\lambda$ . Our investigation of the operator  $B_\lambda$  is split into two parts: first the special case of a circle  $\Sigma$  is treated, and afterwards the results are extended by perturbation arguments to the general case.

#### 4.1. Properties of $B_\lambda$ for a Circle

Throughout this subsection, we assume that  $\Sigma$  is a circle of radius  $R = \frac{L}{2\pi}$ . Without loss of generality we assume that  $\Sigma$  lies in the  $xy$ -plane and is centered at the origin. We will make use of its arc length parametrization

$$\sigma : [0, L] \rightarrow \mathbb{R}^3, \quad \sigma(t) = (R \cos(2\pi t/L), R \sin(2\pi t/L), 0)$$

and occasionally use the formula

$$|\sigma(s) - \sigma(t)| = 2R \sin\left(|s - t| \frac{\pi}{L}\right), \quad s, t \in [0, L], \tag{4.1}$$

which holds for elementary geometric reasons. Furthermore, for  $x = \sigma(t) \in \Sigma$  and  $\delta > 0$  let  $I_\delta^\Sigma(x)$  be the open interval in  $\Sigma$  with center  $x$  and length  $2\delta$  as in (2.6).

Let us first prove the following preliminary lemma. Its proof is partly inspired by [59, Lemma 1].

**Lemma 4.1.** *Let  $\lambda \leq 0$  and  $x \in \Sigma$ . Then the limit*

$$k_\lambda := \lim_{\delta \searrow 0} \left[ \int_{\Sigma \setminus I_\delta^\Sigma(x)} \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) + \frac{\ln \delta}{2\pi} \right]$$

*exists in  $\mathbb{R}$ , is independent of  $x$  and equals*

$$k_\lambda = \int_0^{\frac{\pi}{2}} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)} - 1}{2\pi \sin(s)} ds + \frac{\ln(4R)}{2\pi}.$$

*In particular,  $k_\lambda \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ .*

*Proof.* First of all, it follows from the symmetry of the circle  $\Sigma$  that  $k_\lambda$  is indeed independent of  $x$  (if it exists). Hence, without loss of generality, we can choose  $x = \sigma(0)$ . Using (4.1) and the substitution  $s = \frac{\pi}{L}t$ , we obtain

$$\begin{aligned} \int_{\Sigma \setminus I_\delta^\Sigma(x)} \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) &= \int_\delta^{L-\delta} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(\frac{\pi}{L}t)}}{4\pi \cdot 2R \sin(\frac{\pi}{L}t)} dt \\ &= \int_{\frac{\pi}{L}\delta}^{\pi-\frac{\pi}{L}\delta} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)}}{4\pi \sin(s)} ds, \end{aligned}$$

where we have used  $\frac{\pi}{L} = \frac{1}{2R}$  in the last equality. As  $\sin(\frac{\pi}{2} - s) = \sin(\frac{\pi}{2} + s)$  for all  $s \in \mathbb{R}$  it follows

$$\begin{aligned} &\int_{\Sigma \setminus I_\delta^\Sigma(x)} \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) + \frac{\ln \delta}{2\pi} \\ &= \int_{\frac{\delta}{2R}}^{\frac{\pi}{2}} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)}}{2\pi \sin(s)} ds + \frac{\ln(\frac{\delta}{2R}) - \ln(\frac{\pi}{2}) + \ln(\pi R)}{2\pi} \\ &= \frac{1}{2\pi} \left[ \int_{\frac{\delta}{2R}}^{\frac{\pi}{2}} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)}}{\sin(s)} ds - \int_{\frac{\delta}{2R}}^{\frac{\pi}{2}} \frac{1}{s} ds + \ln(\pi R) \right] \\ &= \frac{1}{2\pi} \left[ \int_{\frac{\delta}{2R}}^{\frac{\pi}{2}} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)} - 1}{\sin(s)} ds + \int_{\frac{\delta}{2R}}^{\frac{\pi}{2}} \frac{1}{\sin(s)} - \frac{1}{s} ds + \ln(\pi R) \right]. \end{aligned} \tag{4.2}$$

With  $\frac{d}{ds} (\ln(\sin(s/2)) - \ln(\cos(s/2))) = \frac{1}{\sin s}$ ,  $s \in (0, \frac{\pi}{2})$ , we get

$$\int_0^{\frac{\pi}{2}} \left( \frac{1}{\sin(s)} - \frac{1}{s} \right) ds = \ln \left( \frac{4}{\pi} \right).$$

Hence, in the limit  $\delta \searrow 0$  the Eq. (4.2) becomes

$$k_\lambda = \int_0^{\frac{\pi}{2}} \frac{e^{-\sqrt{-\lambda} \cdot 2R \sin(s)} - 1}{2\pi \sin(s)} ds + \frac{\ln(4R)}{2\pi}.$$

In particular,  $k_\lambda$  exists and is finite. By monotone convergence, we have

$$\int_0^{\frac{\pi}{2}} \frac{1 - e^{-\sqrt{-\lambda} \cdot 2R \sin(s)}}{\sin(s)} ds \rightarrow \int_0^{\frac{\pi}{2}} \frac{1}{\sin(s)} ds \geq \int_0^{\frac{\pi}{2}} \frac{1}{s} ds = +\infty$$

as  $\lambda \rightarrow -\infty$ , and hence  $k_\lambda \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ . □

As a first step towards the study of the operator  $B_\lambda$  on the circle, we show properties of  $B_0$  in the following lemma.

**Lemma 4.2.** *Consider the operator  $B_0$  in (2.7), i.e.,*

$$(B_0 h)(x) = \lim_{\delta \searrow 0} \left[ \int_{\Sigma \setminus I_\delta^\Sigma(x)} h(y) \frac{1}{4\pi|x-y|} d\sigma(y) + h(x) \frac{\ln \delta}{2\pi} \right], \quad h \in C^{0,1}(\Sigma).$$

*Then the following assertions hold.*

- (i)  $B_0$  is a well-defined, essentially self-adjoint operator in  $L^2(\Sigma)$ .
- (ii)  $\overline{B_0}$  is bounded from above, has a compact resolvent, and its eigenvalues  $\nu_k(0)$ ,  $k = 1, 2, \dots$ , ordered nonincreasingly and counted with multiplicities, are given by

$$\nu_1(0) = \frac{\ln(4R)}{2\pi}, \quad \nu_{2k}(0) = \nu_{2k+1}(0) = \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^k \frac{1}{2j-1}.$$

*Proof.* Let  $h \in C^{0,1}(\Sigma)$ . For every  $x \in \Sigma$ , we can write

$$\begin{aligned} (B_0h)(x) &= \int_{\Sigma} \frac{h(y) - h(x)}{4\pi|x - y|} d\sigma(y) \\ &\quad + h(x) \lim_{\delta \searrow 0} \left[ \int_{\Sigma \setminus I_{\delta}^{\Sigma}(x)} \frac{1}{4\pi|x - y|} d\sigma(y) + \frac{\ln \delta}{2\pi} \right]. \end{aligned}$$

Note that the first integral exists due to the fact that  $h$  is Lipschitz continuous. According to Lemma 4.1 (for  $\lambda = 0$ ) we can write the above equation as

$$(B_0h)(x) = \int_{\Sigma} \frac{h(y) - h(x)}{4\pi|x - y|} d\sigma(y) + h(x) \frac{\ln(4R)}{2\pi}, \tag{4.3}$$

where we have used  $k_0 = \frac{\ln(4R)}{2\pi}$ . It follows directly

$$|(B_0h)(x)| \leq \frac{R}{2} L_h + \frac{\ln(4R)}{2\pi} \|h\|_{\infty},$$

where  $L_h$  is a Lipschitz constant of  $h$ . Thus,  $B_0$  is a well-defined operator in  $L^2(\Sigma)$ .

To show the symmetry of  $B_0$  let  $g, h \in C^{0,1}(\Sigma)$  be arbitrary. Using (4.3), we get

$$\begin{aligned} &\langle B_0h, g \rangle_{L^2(\Sigma)} - \langle h, B_0g \rangle_{L^2(\Sigma)} \\ &= \left\langle \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h, g \right\rangle_{L^2(\Sigma)} - \left\langle h, \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] g \right\rangle_{L^2(\Sigma)} \\ &= \int_{\Sigma} \left( \int_{\Sigma} \frac{h(y) - h(x)}{4\pi|x - y|} d\sigma(y) \right) \overline{g(x)} d\sigma(x) \\ &\quad - \int_{\Sigma} h(y) \overline{\left( \int_{\Sigma} \frac{g(x) - g(y)}{4\pi|x - y|} d\sigma(x) \right)} d\sigma(y) \\ &= \int_{\Sigma} \int_{\Sigma} \frac{h(y)\overline{g(y)} - h(x)\overline{g(x)}}{4\pi|x - y|} d\sigma(y) d\sigma(x) = 0, \end{aligned}$$

where the last equality follows from the fact that the integrand is skew-symmetric with respect to  $x, y$ . Thus,  $B_0$  is symmetric.

Next we calculate the eigenvalues of  $B_0$ ; this will also lead us to the essential self-adjointness of  $B_0$ . Consider the functions  $h_k$  defined by  $h_k(x) = \sin(kt/R)$  with  $x = \sigma(t)$  and  $k \in \mathbb{N}$ . Then by (4.3) and (4.1) we have

$$\begin{aligned} \left( \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h_k \right) (x) &= \int_{\Sigma} \frac{h_k(y) - h_k(x)}{4\pi|x - y|} d\sigma(y) \\ &= \int_0^L \frac{\sin(ks/R) - \sin(kt/R)}{4\pi \cdot 2R \sin\left(\frac{|s-t|}{2R}\right)} ds. \end{aligned}$$

Due to the identity  $\sin(ks/R) - \sin(kt/R) = 2 \sin\left(\frac{ks-kt}{2R}\right) \cos\left(\frac{ks+kt}{2R}\right)$  this leads to

$$\left( \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h_k \right) (x) = \int_0^L \frac{\sin\left(\frac{k(s-t)}{2R}\right) \cos\left(\frac{k(s+t)}{2R}\right)}{4\pi R \sin\left(\frac{|s-t|}{2R}\right)} ds. \tag{4.4}$$

We split the interval of integration into two parts and obtain with the substitution  $z = s - t + L$  for the first integral

$$\begin{aligned} &\int_0^t \frac{\sin\left(\frac{k(s-t)}{2R}\right) \cos\left(\frac{k(s+t)}{2R}\right)}{4\pi R \sin\left(\frac{t-s}{2R}\right)} ds \\ &= \int_{L-t}^L \frac{\sin\left(\frac{k(z-L)}{2R}\right) \cos\left(\frac{k(z-L+2t)}{2R}\right)}{4\pi R \sin\left(\frac{L-z}{2R}\right)} dz \\ &= \int_{L-t}^L \frac{\sin\left(\frac{kz}{2R} - k\pi\right) \cos\left(\frac{kz}{2R} - k\pi + \frac{kt}{R}\right)}{4\pi R \sin\left(\pi - \frac{z}{2R}\right)} dz \\ &= \int_{L-t}^L \frac{\sin\left(\frac{kz}{2R}\right) \cos\left(\frac{kz}{2R} + \frac{kt}{R}\right)}{4\pi R \sin\left(\frac{z}{2R}\right)} dz, \end{aligned} \tag{4.5}$$

where we have used in the last step that  $\sin$  is an odd function and that the formulas  $\sin(x + \pi) = -\sin(x)$  and  $\cos(x + \pi) = -\cos(x)$  hold for all  $x \in \mathbb{R}$ . For the remaining second integral, the substitution  $z = s - t$  yields

$$\int_t^L \frac{\sin\left(\frac{k(s-t)}{2R}\right) \cos\left(\frac{k(s+t)}{2R}\right)}{4\pi R \sin\left(\frac{s-t}{2R}\right)} ds = \int_0^{L-t} \frac{\sin\left(\frac{kz}{2R}\right) \cos\left(\frac{kz}{2R} + \frac{kt}{R}\right)}{4\pi R \sin\left(\frac{z}{2R}\right)} dz. \tag{4.6}$$

With the help of (4.5) and (4.6) and the substitution  $s = z/(2R)$ , the identity (4.4) implies

$$\begin{aligned}
 & \left( \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h_k \right) (x) \\
 &= \int_0^L \frac{\sin\left(\frac{kz}{2R}\right) \cos\left(\frac{kz}{2R} + \frac{kt}{R}\right)}{4\pi R \sin\left(\frac{z}{2R}\right)} dz \\
 &= \int_0^\pi \frac{\sin(ks) \cos\left(ks + \frac{kt}{R}\right)}{2\pi \sin(s)} ds \\
 &= \int_0^\pi \frac{\sin(ks)}{2\pi \sin(s)} \left[ \cos(ks) \cos\left(\frac{kt}{R}\right) - \sin(ks) \sin\left(\frac{kt}{R}\right) \right] ds \\
 &= -\sin\left(\frac{kt}{R}\right) \int_0^\pi \frac{\sin^2(ks)}{2\pi \sin(s)} ds, \tag{4.7}
 \end{aligned}$$

where

$$\int_0^\pi \frac{\sin(ks) \cos(ks)}{2\pi \sin(s)} ds = 0$$

was used in the last step. Furthermore, using  $2 \sin^2(ks) = 1 - \cos(2ks)$  and the indefinite integrals given in [39, 2.526 1. and 2.539 4.], we get

$$\begin{aligned}
 \int_0^\pi \frac{\sin^2(ks)}{2\pi \sin(s)} ds &= \frac{1}{4\pi} \int_0^\pi \frac{1}{\sin(s)} - \frac{\cos(2ks)}{\sin(s)} ds \\
 &= -\frac{1}{2\pi} \sum_{j=1}^k \frac{\cos[(2j-1)s]}{2j-1} \Big|_0^\pi \\
 &= \frac{1}{\pi} \sum_{j=1}^k \frac{1}{2j-1}.
 \end{aligned}$$

Hence, (4.7) yields

$$\left( \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h_k \right) (x) = - \left( \frac{1}{\pi} \sum_{j=1}^k \frac{1}{2j-1} \right) h_k(x). \tag{4.8}$$

By an analogous computation, we see that also

$$\left( \left[ B_0 - \frac{\ln(4R)}{2\pi} \right] \tilde{h}_k \right) (x) = - \left( \frac{1}{\pi} \sum_{j=1}^k \frac{1}{2j-1} \right) \tilde{h}_k(x), \tag{4.9}$$

where  $\tilde{h}_k(x) = \cos(kt/R)$  with  $x = \sigma(t)$ . Moreover, for the constant function  $h(x) = 1$  on  $\Sigma$  we clearly have

$$\left[ B_0 - \frac{\ln(4R)}{2\pi} \right] h = 0. \tag{4.10}$$

Since the functions  $h, h_k, \tilde{h}_k$  are eigenfunctions of  $B_0$  by (4.8), (4.9) and (4.10) and span a dense subspace of  $L^2(\Sigma)$ , it follows that the symmetric operator  $B_0$  is actually essentially self-adjoint in  $L^2(\Sigma)$ . Furthermore, by (4.8), (4.9) and (4.10), the self-adjoint closure  $\overline{B_0}$  has a pure point spectrum and its eigenvalues, counted with multiplicities, are given by  $\nu_k(0), k = 1, 2, \dots$ , in

item (ii). Since these eigenvalues are bounded from above and converge to  $-\infty$  as  $k \rightarrow +\infty$ , it follows that  $\overline{B_0}$  is bounded from above and has a compact resolvent.  $\square$

Let us now turn to the operator  $B_\lambda$  on the circle for general  $\lambda < 0$ .

**Lemma 4.3.** *Let  $\lambda \leq 0$ , let  $\Sigma$  be a circle of radius  $R$  and let  $B_\lambda$  be defined in (2.7). Then the following assertions hold.*

- (i)  $B_\lambda$  is a well-defined, essentially self-adjoint operator in  $L^2(\Sigma)$  and the identity  $\text{dom } \overline{B_\lambda} = \text{dom } \overline{B_0}$  holds.
- (ii)  $\overline{B_\lambda}$  is bounded from above and has a compact resolvent.
- (iii) The eigenvalues  $\nu_k(\lambda)$  of  $\overline{B_\lambda}$ ,  $k = 1, 2, \dots$ , ordered nonincreasingly and counted with multiplicities, satisfy

$$\nu_k(\lambda) = -\frac{\ln k}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty.$$

- (iv) The largest eigenvalue  $\nu_1(\lambda)$  of  $\overline{B_\lambda}$  is given by  $k_\lambda$  in Lemma 4.1. In particular,  $\nu_k(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ ,  $k = 1, 2, \dots$ . The eigenspace corresponding to  $\nu_1(\lambda)$  is given by the constant functions on  $\Sigma$ .

*Proof.* Note first that the operator  $B_\lambda$  can be written as

$$B_\lambda = B_0 - M_\lambda, \tag{4.11}$$

where

$$(M_\lambda h)(x) = \int_\Sigma h(y) \frac{1 - e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y), \quad h \in L^2(\Sigma).$$

The integral operator  $M_\lambda$  has a real, symmetric kernel, which is square integrable since for all  $x, y \in \Sigma$  there exists  $\xi \in [-\sqrt{-\lambda}|x-y|, 0]$  with

$$\left| \frac{1 - e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} \right| = \frac{|e^0 - e^{-\sqrt{-\lambda}|x-y|}|}{4\pi|x-y|} = \frac{e^\xi |0 - (-\sqrt{-\lambda}|x-y||)}{4\pi|x-y|} \leq \frac{\sqrt{-\lambda}}{4\pi}.$$

Thus,  $M_\lambda$  is a compact, self-adjoint operator in  $L^2(\Sigma)$ . Hence, due to Lemma 4.2 and (4.11)  $B_\lambda$  is well defined and essentially self-adjoint in  $L^2(\Sigma)$  with

$$\overline{B_\lambda} = \overline{B_0} - M_\lambda. \tag{4.12}$$

In particular,  $\overline{B_\lambda}$  has a compact resolvent and  $\text{dom } \overline{B_\lambda} = \text{dom } \overline{B_0}$ , which shows (i).

Next, we show that  $\overline{B_\lambda}$  is bounded from above by the number  $k_\lambda$  defined in Lemma 4.1. For every  $h \in C^{0,1}(\Sigma)$  and  $x \in \Sigma$ , we can write

$$(B_\lambda h)(x) = \int_\Sigma [h(y) - h(x)] \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) + k_\lambda \cdot h(x),$$

where again the integral exists due to the Lipschitz continuity of  $h$ . Hence,

$$\begin{aligned} \langle (B_\lambda - k_\lambda)h, h \rangle_{L^2(\Sigma)} &= \int_\Sigma \left( \int_\Sigma [h(y) - h(x)] \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} d\sigma(y) \right) \overline{h(x)} d\sigma(x) \\ &= \int_\Sigma \int_\Sigma [h(y) - h(x)] \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} \overline{h(x)} d\sigma(y) d\sigma(x) \\ &= - \int_\Sigma \int_\Sigma [h(y) - h(x)] \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} \overline{h(y)} d\sigma(y) d\sigma(x), \end{aligned}$$

where in the last step we first changed the roles of  $x$  and  $y$  and then the order of integration. Addition of the last two lines yields

$$\begin{aligned} 2 \langle (B_\lambda - k_\lambda)h, h \rangle_{L^2(\Sigma)} &= \int_\Sigma \int_\Sigma [h(y) - h(x)] \frac{e^{-\sqrt{-\lambda}|x-y|}}{4\pi|x-y|} [\overline{h(x)} - \overline{h(y)}] d\sigma(y) d\sigma(x) \\ &\leq 0 \end{aligned}$$

and, hence,  $\langle B_\lambda h, h \rangle_{L^2(\Sigma)} \leq k_\lambda \langle h, h \rangle_{L^2(\Sigma)}$  for all  $h \in C^{0,1}(\Sigma)$ , with equality if and only if  $h$  is constant, that is,  $B_\lambda$  (and, thus,  $\overline{B_\lambda}$ ) is bounded from above by  $k_\lambda$ , which shows (ii). Moreover, it follows  $\nu_1(\lambda) = k_\lambda$ . By Lemma 4.1 this implies  $\nu_1(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$  and thus  $\nu_k(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$  for all  $k$ . This finishes the proof of (iv).

It remains to verify the asymptotic behavior of the eigenvalue  $\nu_k(\lambda)$  for  $k \rightarrow +\infty$  as claimed in (iii). According to [1, Equation 4.1.32], we have

$$\sum_{j=1}^k \frac{1}{j} = \ln(k) + \gamma + o(1) \quad \text{as } k \rightarrow +\infty,$$

where  $\gamma \approx 0.577216$  denotes the Euler–Mascheroni constant. Hence,

$$\begin{aligned} \sum_{j=1}^k \frac{1}{2j-1} &= \sum_{j=1}^{2k} \frac{1}{j} - \frac{1}{2} \sum_{j=1}^k \frac{1}{j} = \ln(2k) + \gamma - \frac{\ln(k) + \gamma}{2} + o(1) \\ &= \frac{\gamma}{2} + \frac{\ln(4k)}{2} + o(1) \quad \text{as } k \rightarrow +\infty. \end{aligned}$$

By Lemma 4.2 (ii) for the eigenvalues of  $\overline{B_0}$  this implies

$$\begin{aligned} \nu_{2k}(0) &= \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^k \frac{1}{2j-1} = \frac{\ln(4R)}{2\pi} - \frac{\gamma}{2\pi} - \frac{\ln(4k)}{2\pi} + o(1) \\ &= -\frac{\ln k}{2\pi} + \frac{\ln R - \gamma}{2\pi} + o(1) = -\frac{\ln(2k)}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty \end{aligned} \tag{4.13}$$

and consequently

$$\begin{aligned} \nu_{2k+1}(0) = \nu_{2k}(0) &= -\frac{\ln(2k+1) - \ln(\frac{2k+1}{2k})}{2\pi} + O(1) \\ &= -\frac{\ln(2k+1)}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty. \end{aligned} \tag{4.14}$$



From (4.12), we conclude with the help of the min-max principle

$$\nu_k(0) - \|M_\lambda\| \leq \nu_k(\lambda) \leq \nu_k(0) + \|M_\lambda\|, \quad k = 1, 2, \dots$$

The latter together with (4.13) and (4.14) implies

$$\nu_k(\lambda) = \nu_k(0) + O(1) = -\frac{\ln k}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty,$$

which completes the proof of the lemma. □

**4.2. Properties of  $B_\lambda$  in the General Case**

In this subsection,  $\Sigma$  is an arbitrary compact, closed, regular  $C^2$ -curve in  $\mathbb{R}^3$  of length  $L$  without self-intersections. In the following, we explore properties of  $B_\lambda$  using the results of the previous subsection for the case of a circle. This will be done by a perturbation argument.

Let  $\mathcal{T}$  be a circle in  $\mathbb{R}^3$  with radius  $R = \frac{L}{2\pi}$  which is parametrized with respect to the arc length by a function  $\tau : [0, L] \rightarrow \mathbb{R}^3$ . To distinguish the operators  $B_\lambda$  on  $\Sigma$  from those on the circle  $\mathcal{T}$  we denote the latter by  $B_\lambda^\mathcal{T}$ . Moreover, recall that  $\sigma : [0, L] \rightarrow \mathbb{R}^3$  is an arc length parametrization of  $\Sigma$ . We define an operator  $D_\lambda$  by

$$(D_\lambda h)(\sigma(t)) = \int_0^L h(\sigma(s)) \left[ \frac{e^{-\sqrt{-\lambda}|\sigma(t)-\sigma(s)|}}{4\pi|\sigma(t)-\sigma(s)|} - \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tau(s)|}}{4\pi|\tau(t)-\tau(s)|} \right] ds \quad (4.15)$$

for  $h \in L^2(\Sigma)$ . Furthermore, let  $J : L^2(\Sigma) \rightarrow L^2(\mathcal{T})$  be the unitary operator defined by

$$Jh = h \circ \sigma \circ \tau^{-1}, \quad h \in L^2(\Sigma). \quad (4.16)$$

Our studies of  $B_\lambda$  will rely on the following properties of  $D_\lambda$ .

**Lemma 4.4.** *For each  $\lambda \leq 0$ , the operator  $D_\lambda$  in (4.15) is well defined, compact and self-adjoint in  $L^2(\Sigma)$ , and  $\|D_\lambda\| \leq C$  holds for all  $\lambda \leq 0$  and some  $C > 0$  which is independent of  $\lambda$ . In the special case  $\lambda = 0$ , the estimate*

$$\|D_0\| \leq d_\Sigma \quad (4.17)$$

holds with  $d_\Sigma$  given in (3.3). Moreover, the relation

$$B_\lambda = D_\lambda + J^* B_\lambda^\mathcal{T} J \quad (4.18)$$

is satisfied for all  $\lambda \leq 0$ .

*Proof.* To study the integral in the definition (4.15) of  $D_\lambda$ , we identify the parametrizations  $\sigma, \tau$  of  $\Sigma$  and  $\mathcal{T}$ , respectively, with their  $L$ -periodic continuations to all of  $\mathbb{R}$ . Let  $s, t \in \mathbb{R}$  with  $|s - t| \leq \frac{L}{2}$ . Define  $f : (0, \infty) \rightarrow \mathbb{R}$  via  $f(z) = \frac{e^{-\sqrt{-\lambda}z}}{4\pi z}$  for  $z > 0$ . Then

$$f'(z) = \frac{-\sqrt{-\lambda}e^{-\sqrt{-\lambda}z}4\pi z - e^{-\sqrt{-\lambda}z}4\pi}{(4\pi z)^2} = -e^{-\sqrt{-\lambda}z} \frac{\sqrt{-\lambda}z + 1}{4\pi z^2}, \quad (4.19)$$

from which it follows that  $f'$  is monotonously nondecreasing on  $(0, \infty)$  and, thus,  $|f'|$  is monotonously nonincreasing on  $(0, \infty)$ . Hence, with

$$\zeta_{\min} = \min \{|\sigma(t) - \sigma(s)|, |\tau(t) - \tau(s)|\}$$

it follows

$$\begin{aligned} & \left| \frac{e^{-\sqrt{-\lambda}|\sigma(t)-\sigma(s)}}{4\pi|\sigma(t)-\sigma(s)} - \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tau(s)}}{4\pi|\tau(t)-\tau(s)} \right| \\ & \leq |f'(\zeta_{\min})| \cdot \left| |\sigma(t)-\sigma(s)| - |\tau(t)-\tau(s)| \right|. \end{aligned} \tag{4.20}$$

Note that there exist  $\varepsilon_\sigma > 0$  and  $\varepsilon_\tau > 0$  such that for all  $s, t \in \mathbb{R}$  with  $|s-t| \leq \frac{t}{2}$

$$|\sigma(s) - \sigma(t)| \geq \varepsilon_\sigma |s - t| \quad \text{and} \quad |\tau(s) - \tau(t)| \geq \varepsilon_\tau |s - t|$$

holds. With  $\varepsilon := \min\{\varepsilon_\sigma, \varepsilon_\tau\} > 0$ , the estimate (4.20) can be simplified to

$$\begin{aligned} & \left| \frac{e^{-\sqrt{-\lambda}|\sigma(t)-\sigma(s)}}{4\pi|\sigma(t)-\sigma(s)} - \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tau(s)}}{4\pi|\tau(t)-\tau(s)} \right| \\ & \leq |f'(\varepsilon|s-t|)| \left| |\sigma(t)-\sigma(s)| - |\tau(t)-\tau(s)| \right|. \end{aligned} \tag{4.21}$$

Recall that  $\Sigma$  is a  $C^2$ -curve. Hence, we get with Taylor’s theorem (for each component) for some suitable  $\zeta_1, \zeta_2$  and  $\zeta_3$

$$\sigma(t) = \begin{bmatrix} \sigma_1(t) \\ \sigma_2(t) \\ \sigma_3(t) \end{bmatrix} = \sigma(s) + \sigma'(s)(t-s) + \begin{bmatrix} \sigma''_1(\zeta_1) \\ \sigma''_2(\zeta_2) \\ \sigma''_3(\zeta_3) \end{bmatrix} \frac{(t-s)^2}{2}.$$

With  $C_\sigma := \sqrt{\|\sigma''_1\|_\infty^2 + \|\sigma''_2\|_\infty^2 + \|\sigma''_3\|_\infty^2}$  and  $|\sigma'(s)| = 1$  it follows

$$|\sigma(t) - \sigma(s)| \leq |\sigma'(s)| \cdot |t-s| + \left| \begin{bmatrix} \sigma''_1(\zeta_1) \\ \sigma''_2(\zeta_2) \\ \sigma''_3(\zeta_3) \end{bmatrix} \right| \frac{(t-s)^2}{2} \leq |t-s| + \frac{C_\sigma}{2}|t-s|^2.$$

Analogously, we get with  $C_\tau := \sqrt{\|\tau''_1\|_\infty^2 + \|\tau''_2\|_\infty^2 + \|\tau''_3\|_\infty^2}$

$$|\tau(t) - \tau(s)| \geq |\tau'(s)| \cdot |t-s| - \left| \begin{bmatrix} \tau''_1(\xi_1) \\ \tau''_2(\xi_2) \\ \tau''_3(\xi_3) \end{bmatrix} \right| \frac{(t-s)^2}{2} \geq |t-s| - \frac{C_\tau}{2}|t-s|^2$$

for some suitable  $\xi_1, \xi_2$  and  $\xi_3$ . Hence,

$$|\sigma(t) - \sigma(s)| - |\tau(t) - \tau(s)| \leq \frac{C_\sigma + C_\tau}{2}|t-s|^2.$$

By changing the roles of  $\sigma$  and  $\tau$ , we observe

$$\left| |\sigma(t) - \sigma(s)| - |\tau(t) - \tau(s)| \right| \leq \frac{C_\sigma + C_\tau}{2}|t-s|^2. \tag{4.22}$$

Note that  $e^{-x}(x+1) \leq 1$  for  $x \geq 0$ . Together with (4.19), (4.22) and

$$\tilde{C} := \frac{C_\sigma + C_\tau}{8\pi e^2}$$

the estimate (4.21) implies

$$\begin{aligned} & \left| \frac{e^{-\sqrt{-\lambda}|\sigma(t)-\sigma(s)|}}{4\pi|\sigma(t)-\sigma(s)|} - \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tau(s)|}}{4\pi|\tau(t)-\tau(s)|} \right| \\ & \leq \tilde{C}e^{-\sqrt{-\lambda}\varepsilon|s-t|} \left[ \sqrt{-\lambda}\varepsilon|s-t| + 1 \right] \leq \tilde{C} \end{aligned} \tag{4.23}$$

for all  $s, t \in \mathbb{R}$  with  $|s - t| \leq \frac{L}{2}$ . For arbitrary  $s, t \in \mathbb{R}$ , there exists  $k \in \mathbb{Z}$  such that  $|(s + kL) - t| \leq \frac{L}{2}$ . As  $\sigma$  and  $\tau$  are  $L$ -periodic it follows that (4.23) holds for all  $s, t \in \mathbb{R}$ . From (4.23), we conclude that the integral kernel of the operator  $D_\lambda$  is bounded with a bound  $\tilde{C}$  independent of  $\lambda$ . Thus, with  $C = \tilde{C}L$ , the definition of  $D_\lambda$  in (4.15) and estimate (4.23) follows

$$\begin{aligned} \|D_\lambda h\|_{L^2(\Sigma)}^2 & \leq \|h\|_{L^2(\Sigma)}^2 \int_0^L \int_0^L \left| \frac{e^{-\sqrt{-\lambda}|\sigma(t)-\sigma(s)|}}{4\pi|\sigma(t)-\sigma(s)|} - \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tau(s)|}}{4\pi|\tau(t)-\tau(s)|} \right|^2 ds dt \\ & \leq C^2 \|h\|_{L^2(\Sigma)}^2 \end{aligned}$$

for all  $h \in L^2(\Sigma)$  and  $C$  does not depend on  $\lambda$ . In particular,  $D_\lambda$  is a well-defined, compact operator in  $L^2(\Sigma)$  whose operator norm can be estimated by a constant independent of  $\lambda$ . Since the integral kernel of  $D_\lambda$  is real and symmetric, it follows that  $D_\lambda$  is self-adjoint. For  $\lambda = 0$ , the estimate (4.17) follows immediately from the definition of  $D_\lambda$ .

To verify the relation (4.18) observe that  $h \in C^{0,1}(\Sigma)$  if and only if  $\tilde{h} := Jh \in C^{0,1}(T)$  and in this case

$$(J^* B_\lambda^T Jh)(x) = \lim_{\delta \searrow 0} \left[ \int_{T \setminus I_\delta^T(\tau(t))} \tilde{h}(\tilde{y}) \frac{e^{-\sqrt{-\lambda}|\tau(t)-\tilde{y}|}}{4\pi|\tau(t)-\tilde{y}|} d\sigma(\tilde{y}) + \tilde{h}(\tau(t)) \frac{\ln \delta}{2\pi} \right]$$

for every  $h \in C^{0,1}(\Sigma)$  and  $x = \sigma(t) \in \Sigma$ . This identity and the definitions of  $B_\lambda$  and  $D_\lambda$  lead to the relation (4.18). □

Now we are in the position to prove all properties of  $B_\lambda$  which are required for the proofs of the main results of this paper.

**Proposition 4.5.** *Let  $\lambda \leq 0$  and let  $B_\lambda$  be given in (2.7). Then the following assertions hold.*

- (i)  $B_\lambda$  is a well-defined, essentially self-adjoint operator in  $L^2(\Sigma)$  and the identity  $\text{dom } \overline{B_\lambda} = \text{dom } \overline{B_0}$  holds.
- (ii)  $\overline{B_\lambda}$  is bounded from above and has a compact resolvent.
- (iii) The eigenvalues  $\nu_k(\lambda)$  of  $\overline{B_\lambda}$ ,  $k = 1, 2, \dots$ , ordered nonincreasingly and counted with multiplicities, satisfy

$$\nu_k(\lambda) = -\frac{\ln k}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty.$$

- (iv) For every  $k \in \mathbb{N}$ , the function  $\lambda \mapsto \nu_k(\lambda)$  is continuous and strictly increasing on the interval  $(-\infty, 0]$  and  $\nu_k(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ .

*Proof.* Let  $D_\lambda$  be given in (4.15) and let  $J : L^2(\Sigma) \rightarrow L^2(\mathcal{T})$  be the unitary operator in (4.16). Since  $D_\lambda$  is self-adjoint and compact in  $L^2(\Sigma)$  by Lemma 4.4, the assertions in (i) and (ii) follow directly from (4.18) and Lemma 4.3 (i) and (ii). Furthermore, by (4.18), Lemma 4.3 (ii) and (iv), and Lemma 4.4, there exists  $C > 0$  independent of  $\lambda$  such that for  $h \in \text{dom } \overline{B}_\lambda$  we have

$$\begin{aligned} \langle \overline{B}_\lambda h, h \rangle_{L^2(\Sigma)} &= \langle D_\lambda h, h \rangle_{L^2(\Sigma)} + \left\langle \overline{B}_\lambda^\mathcal{T} Jh, Jh \right\rangle_{L^2(\mathcal{T})} \\ &\leq \|D_\lambda\| \cdot \|h\|_{L^2(\Sigma)}^2 + k_\lambda \|Jh\|_{L^2(\mathcal{T})}^2 \\ &\leq (C + k_\lambda) \|h\|_{L^2(\Sigma)}^2, \end{aligned} \tag{4.24}$$

where  $k_\lambda$  is given in Lemma 4.1. Since  $k_\lambda \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$  by Lemma 4.1, we conclude from (4.24) that  $\nu_k(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$  for each  $k$ . From (4.18) and the min-max principle, it follows

$$\nu_k(\lambda) - C \leq \nu_k^\mathcal{T}(\lambda) \leq \nu_k(\lambda) + C, \quad k = 1, 2, \dots,$$

where  $\nu_k^\mathcal{T}(\lambda)$  denotes the  $k$ th eigenvalue of  $\overline{B}_\lambda^\mathcal{T}$ . We obtain with the help of Lemma 4.3 (iii) that

$$\nu_k(\lambda) = \nu_k^\mathcal{T}(\lambda) + O(1) = -\frac{\ln k}{2\pi} + O(1) \quad \text{as } k \rightarrow +\infty.$$

This proves the assertion (iii).

To show the remaining assertions in (iv), let  $\lambda, \mu \leq 0$  and define the operator  $D_{\lambda,\mu} : L^2(\Sigma) \rightarrow L^2(\Sigma)$  by

$$(D_{\lambda,\mu}h)(x) = \int_\Sigma h(y) \frac{e^{-\sqrt{-\lambda}|x-y|} - e^{-\sqrt{-\mu}|x-y|}}{4\pi|x-y|} d\sigma(y), \quad h \in L^2(\Sigma).$$

As  $B_\lambda h - B_\mu h = D_{\lambda,\mu}h$  for all  $h \in C^{0,1}(\Sigma)$ , it follows that

$$\overline{B}_\lambda h = \overline{B}_\mu h + D_{\lambda,\mu}h, \quad h \in \text{dom } \overline{B}_\lambda. \tag{4.25}$$

As in the proof of Lemma 4.3 one shows that  $D_{\lambda,\mu}$  is a compact, self-adjoint operator with

$$\|D_{\lambda,\mu}\| \leq \frac{|\sqrt{-\lambda} - \sqrt{-\mu}|}{4\pi} L.$$

In particular,  $\|D_{\lambda,\mu}\| \rightarrow 0$  as  $\lambda \rightarrow \mu$ . From this and (4.25), it follows with the min-max principle that  $\nu_k(\lambda) \rightarrow \nu_k(\mu)$  for all  $k$ , that is, all the functions  $\lambda \mapsto \nu_k(\lambda)$  are continuous.

For the strict monotonicity, let  $\lambda, \mu < 0$ . If  $h \in \text{dom } B_\lambda = \text{dom } B_\mu$ , it follows from the definition of  $\gamma_\lambda$  and  $\gamma_\mu$  in (2.3) that

$$\begin{aligned} \gamma_\lambda h - \gamma_\mu h &= (-\Delta - \lambda)^{-1}(h\delta_\Sigma) - (-\Delta - \mu)^{-1}(h\delta_\Sigma) \\ &= (\lambda - \mu)(-\Delta - \lambda)^{-1}(-\Delta - \mu)^{-1}(h\delta_\Sigma), \end{aligned} \tag{4.26}$$

in particular,  $\gamma_\lambda h - \gamma_\mu h \in H^2(\mathbb{R}^3)$ . Note also that  $\gamma_\lambda - \gamma_\mu$  is continuous from  $L^2(\Sigma)$  to  $H^2(\mathbb{R}^3)$  since  $\gamma_\lambda - \gamma_\mu$  is defined on  $L^2(\Sigma)$  and is closed as a mapping from  $L^2(\Sigma)$  to  $H^2(\mathbb{R}^3)$ . According to Lemma 2.1, we have

$$(\gamma_\lambda h - \gamma_\mu h)(x) = \int_\Sigma h(s) \frac{e^{-\sqrt{-\lambda}|x-s|} - e^{-\sqrt{-\mu}|x-s|}}{4\pi|x-s|} ds \tag{4.27}$$

for almost all  $x \in \mathbb{R}^3 \setminus \Sigma$ . As the integral in (4.27) is continuous with respect to  $x$  we obtain (4.27) for all  $x \in \mathbb{R}^3$ . In particular,

$$\begin{aligned} (\gamma_\lambda h - \gamma_\mu h)|_\Sigma(x) &= \int_\Sigma h(s) \frac{e^{-\sqrt{-\lambda}|x-s|} - e^{-\sqrt{-\mu}|x-s|}}{4\pi|x-s|} ds \\ &= (B_\lambda h - B_\mu h)(x) \end{aligned} \tag{4.28}$$

for all  $x \in \Sigma$  and  $h \in C^{0,1}(\Sigma) = \text{dom } B_\lambda = \text{dom } B_\mu$ . If  $h \in \text{dom } \overline{B_\lambda} = \text{dom } \overline{B_\mu}$ , we can choose a sequence  $(h_n) \subset \text{dom } B_\lambda = \text{dom } B_\mu$  such that  $h_n \rightarrow h$  and  $B_\lambda h_n \rightarrow \overline{B_\lambda} h$ . Due to (4.28) and (4.26), we observe

$$\begin{aligned} B_\lambda h_n &= B_\mu h_n + (\gamma_\lambda h_n - \gamma_\mu h_n)|_\Sigma \\ &= B_\mu h_n + ((\lambda - \mu)(-\Delta - \lambda)^{-1}(-\Delta - \mu)^{-1}(h_n \delta_\Sigma))|_\Sigma. \end{aligned}$$

Since the mapping  $h \mapsto h\delta_\Sigma$  is continuous from  $L^2(\Sigma)$  to  $H^{-2}(\mathbb{R}^3)$  (see (2.2)),  $-\Delta - \lambda$  is an isomorphism between  $H^s(\mathbb{R}^3)$  and  $H^{s-2}(\mathbb{R}^3)$  for all  $s \in \mathbb{R}$ , and the trace map is continuous from  $H^2(\mathbb{R}^3)$  to  $L^2(\Sigma)$ , we conclude

$$\overline{B_\lambda} h = \lim_{n \rightarrow \infty} B_\mu h_n + ((\lambda - \mu)(-\Delta - \lambda)^{-1}(-\Delta - \mu)^{-1}(h\delta_\Sigma))|_\Sigma$$

and hence the limit  $\lim_{n \rightarrow \infty} B_\mu h_n$  exists and equals  $\overline{B_\mu} h$ . Using the continuity of  $\gamma_\lambda - \gamma_\mu$  as a mapping from  $L^2(\Sigma)$  to  $H^2(\mathbb{R}^3)$ , the continuity of the trace and (4.28), we observe

$$\begin{aligned} (\gamma_\lambda h - \gamma_\mu h)|_\Sigma &= \lim_{n \rightarrow \infty} (\gamma_\lambda h_n - \gamma_\mu h_n)|_\Sigma \\ &= \lim_{n \rightarrow \infty} (B_\lambda h_n - B_\mu h_n) \\ &= \overline{B_\lambda} h - \overline{B_\mu} h \end{aligned} \tag{4.29}$$

for all  $h \in \text{dom } \overline{B_\lambda} = \text{dom } \overline{B_\mu}$ . From (4.29), (4.26) and (2.2), we obtain

$$\begin{aligned} &\langle (\overline{B_\lambda} - \overline{B_\mu}) h, h \rangle_{L^2(\Sigma)} \\ &= \langle (\gamma_\lambda h - \gamma_\mu h)|_\Sigma, h \rangle_{L^2(\Sigma)} \\ &= \langle [(\lambda - \mu)(-\Delta - \lambda)^{-1}(-\Delta - \mu)^{-1}(h\delta_\Sigma)]|_\Sigma, h \rangle_{L^2(\Sigma)} \\ &= (\lambda - \mu) \langle (-\Delta - \lambda)^{-1}(-\Delta - \mu)^{-1}(h\delta_\Sigma), h\delta_\Sigma \rangle_{2,-2} \\ &= (\lambda - \mu) \langle (-\Delta - \mu)^{-1}(h\delta_\Sigma), (-\Delta - \lambda)^{-1}(h\delta_\Sigma) \rangle_{L^2(\Sigma)}. \end{aligned}$$

Hence,

$$\begin{aligned} \lim_{\mu \rightarrow \lambda} \frac{\langle \overline{B_\lambda} h, h \rangle_{L^2(\Sigma)} - \langle \overline{B_\mu} h, h \rangle_{L^2(\Sigma)}}{\lambda - \mu} &= \|(-\Delta - \lambda)^{-1}(h\delta_\Sigma)\|_{L^2(\Sigma)}^2 \\ &= \|\gamma_\lambda h\|_{L^2(\Sigma)}^2. \end{aligned}$$

Since  $\gamma_\lambda$  is an injective operator it follows that the function  $\lambda \mapsto \langle \overline{B_\lambda}h, h \rangle_{L^2(\Sigma)}$  is strictly increasing on  $(-\infty, 0)$ , as its derivative is positive, i.e.,

$$\langle \overline{B_\lambda}h, h \rangle_{L^2(\Sigma)} < \langle \overline{B_\mu}h, h \rangle_{L^2(\Sigma)}$$

whenever  $\lambda < \mu < 0$ . From this and the min-max principle for  $\lambda < \mu < 0$ , we obtain

$$\begin{aligned} -\nu_k(\lambda) &= \min_{\substack{U \subseteq \text{dom } \overline{B_\lambda} \\ \dim U = k}} \max_{\substack{h \in U \\ \|h\|=1}} \langle -\overline{B_\lambda}h, h \rangle_{L^2(\Sigma)} \\ &> \min_{\substack{U \subseteq \text{dom } \overline{B_\mu} \\ \dim U = k}} \max_{\substack{h \in U \\ \|h\|=1}} \langle -\overline{B_\mu}h, h \rangle_{L^2(\Sigma)} = -\nu_k(\mu), \end{aligned}$$

where we have used that the operators  $-\overline{B_\lambda}$  and  $-\overline{B_\mu}$  are bounded from below; cf. (ii). Thus,  $\nu_k(\lambda) < \nu_k(\mu)$  for  $\lambda < \mu < 0$  and by continuity the same holds in the case  $\lambda < \mu = 0$ . This proves the remaining assertion in (iv).  $\square$

### 4.3. Well-definedness of the Generalized Trace

In this subsection, we verify that the definition of the generalized trace  $u|_\Sigma$  in (2.8) is independent of the choice of  $\lambda < 0$ . Observe first that if

$$u = u_c + \gamma_\lambda h, \quad u_c \in H^2(\mathbb{R}^3), \quad h \in \text{dom } \overline{B_\lambda}, \tag{4.30}$$

for some  $\lambda < 0$  then  $h \in \text{dom } \overline{B_\mu}$  for any  $\mu < 0$  by Proposition 4.5 (i) and

$$u = v_c + \gamma_\mu h, \quad \text{where } v_c := u_c + \gamma_\lambda h - \gamma_\mu h. \tag{4.31}$$

It follows as in (4.26) that  $\gamma_\lambda h - \gamma_\mu h$  belongs to  $H^2(\mathbb{R}^3)$ , and hence also  $v_c \in H^2(\mathbb{R}^3)$ . Thus, if  $u$  admits the decomposition (4.30) with respect to some  $\lambda < 0$ , then  $u$  admits the decomposition (4.31) with respect to any  $\mu < 0$ . Note also that for fixed  $\lambda < 0$  both elements  $u_c$  and  $h$  in the decomposition (4.30) are unique.

Let now  $\lambda, \mu < 0$  and assume that

$$u = u_c + \gamma_\lambda h = v_c + \gamma_\mu k \tag{4.32}$$

with  $u_c, v_c \in H^2(\mathbb{R}^3)$  and  $h, k \in \text{dom } \overline{B_\lambda} = \text{dom } \overline{B_\mu}$ . Then it follows from the above considerations and the uniqueness of the decompositions in (4.32) that

$$v_c = u_c + \gamma_\lambda h - \gamma_\mu h \quad \text{and} \quad h = k. \tag{4.33}$$

Using (4.29), it follows from (4.33) that

$$\begin{aligned} v_c|_\Sigma + \overline{B_\mu}k &= (u_c + \gamma_\lambda h - \gamma_\mu h)|_\Sigma + \overline{B_\mu}h \\ &= u_c|_\Sigma + (\overline{B_\lambda}h - \overline{B_\mu}h) + \overline{B_\mu}h \\ &= u_c|_\Sigma + \overline{B_\lambda}h. \end{aligned}$$

This shows that the definition of the generalized trace in (2.8) is independent of the choice of  $\lambda$ .

## 5. Proofs of the Main Results

In this section, we provide the complete proofs of the results in Sect. 3.

**5.1. Proof of Theorem 3.1**

We start by proving assertion (i). Assume first that  $\lambda \in \sigma_p(-\Delta_{\Sigma,\alpha})$  for some  $\lambda < 0$ , let  $u \in \ker(-\Delta_{\Sigma,\alpha} - \lambda)$ ,  $u \neq 0$ , and write  $u = u_c + \gamma_\lambda h$  with  $u_c \in H^2(\mathbb{R}^3)$  and  $h \in \text{dom } \overline{B_\lambda}$ . Using the definition of  $\gamma_\lambda$  in (2.3), we obtain

$$\begin{aligned} 0 &= (-\Delta_{\Sigma,\alpha} - \lambda)(u_c + \gamma_\lambda h) \\ &= (-\Delta - \lambda)(u_c + \gamma_\lambda h) - \frac{1}{\alpha} u|_\Sigma \cdot \delta_\Sigma \\ &= (-\Delta - \lambda)u_c + \frac{1}{\alpha}(\alpha h - u|_\Sigma)\delta_\Sigma. \end{aligned}$$

Since  $(-\Delta - \lambda)u_c \in L^2(\mathbb{R}^3)$  it follows  $u_c = 0$ . In particular,  $0 \neq u = \gamma_\lambda h$ , which implies  $h \neq 0$ . Moreover,

$$\alpha h = u|_\Sigma = (\gamma_\lambda h)|_\Sigma = \overline{B_\lambda} h,$$

that is,  $h \in \ker(\alpha - \overline{B_\lambda})$ . Since  $u = \gamma_\lambda h$ , it follows

$$\ker(-\Delta_{\Sigma,\alpha} - \lambda) \subseteq \gamma_\lambda (\ker(\alpha - \overline{B_\lambda})).$$

Conversely, if  $h \in \ker(\alpha - \overline{B_\lambda})$ ,  $h \neq 0$ , for some  $\lambda < 0$  set  $u = \gamma_\lambda h$ . Since  $\gamma_\lambda$  is injective, we obtain  $u \neq 0$  and

$$u|_\Sigma = (\gamma_\lambda h)|_\Sigma = \overline{B_\lambda} h = \alpha h,$$

and hence

$$(\mathcal{A}_\alpha - \lambda)u = (-\Delta - \lambda)\gamma_\lambda h - \frac{1}{\alpha} u|_\Sigma \cdot \delta_\Sigma = h\delta_\Sigma - h\delta_\Sigma = 0.$$

From this, we conclude  $(-\Delta_{\Sigma,\alpha} - \lambda)u = 0$ . Thus,

$$\gamma_\lambda (\ker(\alpha - \overline{B_\lambda})) \subseteq \ker(-\Delta_{\Sigma,\alpha} - \lambda)$$

and  $\lambda \in \sigma_p(-\Delta_{\Sigma,\alpha})$ . Since  $\gamma_\lambda$  is continuous as a mapping from  $L^2(\Sigma)$  to  $L^2(\mathbb{R}^3)$ , it follows that  $\gamma_\lambda$  is an isomorphism between the spaces  $\ker(\alpha - \overline{B_\lambda})$  and  $\ker(-\Delta_{\Sigma,\alpha} - \lambda)$ .

Next, we verify the resolvent formula (3.1) in (ii) and, simultaneously, the self-adjointness of  $-\Delta_{\Sigma,\alpha}$ . In the following, for a given  $\alpha \neq 0$  fix  $\lambda_0 < 0$  such that  $\alpha \notin \sigma_p(\overline{B_{\lambda_0}})$ ; this is possible according to Proposition 4.5 (iv). By item (i), we have

$$\ker(-\Delta_{\Sigma,\alpha} - \lambda_0) = \{0\}.$$

Let now  $v \in L^2(\mathbb{R}^3)$  be arbitrary and define

$$u = (-\Delta_{\text{free}} - \lambda_0)^{-1} v + \gamma_{\lambda_0} (\alpha - \overline{B_{\lambda_0}})^{-1} \gamma_{\lambda_0}^* v \in L^2(\mathbb{R}^3), \tag{5.1}$$

and note that  $(\alpha - \overline{B_{\lambda_0}})^{-1}$  is a bounded, self-adjoint operator in  $L^2(\Sigma)$ ; cf. Proposition 4.5 (i) and (ii). Furthermore, as  $(-\Delta_{\text{free}} - \lambda_0)^{-1} v \in H^2(\mathbb{R}^3)$  and  $(\alpha - \overline{B_{\lambda_0}})^{-1} \gamma_{\lambda_0}^* v \in \text{dom } \overline{B_{\lambda_0}}$ , the trace  $u|_\Sigma$  is well defined in the sense of (2.8).

Making use of (2.5), we compute

$$\begin{aligned}
 u|_{\Sigma} &= ((-\Delta_{\text{free}} - \lambda_0)^{-1}v)|_{\Sigma} + \overline{B_{\lambda_0}}(\alpha - \overline{B_{\lambda_0}})^{-1}\gamma_{\lambda_0}^*v \\
 &= \left(I + \overline{B_{\lambda_0}}(\alpha - \overline{B_{\lambda_0}})^{-1}\right)\gamma_{\lambda_0}^*v \\
 &= \alpha(\alpha - \overline{B_{\lambda_0}})^{-1}\gamma_{\lambda_0}^*v.
 \end{aligned}
 \tag{5.2}$$

From (2.3), (5.2) and the definition of  $u$  in (5.1), we then conclude

$$\begin{aligned}
 (\mathcal{A}_{\alpha} - \lambda_0)u &= (-\Delta - \lambda_0)u - \frac{1}{\alpha}u|_{\Sigma} \cdot \delta_{\Sigma} \\
 &= v + \left((\alpha - \overline{B_{\lambda_0}})^{-1}\gamma_{\lambda_0}^*v\right) \cdot \delta_{\Sigma} - \frac{1}{\alpha}u|_{\Sigma} \cdot \delta_{\Sigma} \\
 &= v
 \end{aligned}$$

and hence  $\mathcal{A}_{\alpha}u = v + \lambda_0u \in L^2(\mathbb{R}^3)$ . Thus, we have  $u \in \text{dom}(-\Delta_{\Sigma, \alpha})$  and

$$(-\Delta_{\Sigma, \alpha} - \lambda_0)^{-1}v = u = (-\Delta_{\text{free}} - \lambda_0)^{-1}v + \gamma_{\lambda_0}(\alpha - \overline{B_{\lambda_0}})^{-1}\gamma_{\lambda_0}^*v.$$

Since  $v \in L^2(\mathbb{R}^3)$  was arbitrary, the identity (3.1) follows for  $\lambda_0$ . In particular, since  $(\alpha - \overline{B_{\lambda_0}})^{-1}$  is a bounded, self-adjoint operator in  $L^2(\Sigma)$ , it follows that  $(-\Delta_{\Sigma, \alpha} - \lambda_0)^{-1}$  is bounded and self-adjoint in  $L^2(\mathbb{R}^3)$ . This implies that  $\lambda_0 \in \rho(-\Delta_{\Sigma, \alpha})$  and that  $-\Delta_{\Sigma, \alpha}$  is a self-adjoint operator in  $L^2(\mathbb{R}^3)$ .

Assume now that  $\lambda \in \rho(-\Delta_{\Sigma, \alpha}) \cap (-\infty, 0)$  is arbitrary. Then  $\alpha \in \rho(\overline{B_{\lambda}})$  by item (i) and Proposition 4.5 (ii) and the above arguments with  $\lambda_0$  replaced by  $\lambda$  yield the resolvent formula (3.1) for all  $\lambda \in \rho(-\Delta_{\Sigma, \alpha}) \cap (-\infty, 0)$ . The identity (3.1) also implies

$$\begin{aligned}
 \|(-\Delta_{\Sigma, \alpha} - \lambda)^{-1} - (-\Delta_{\text{free}} - \lambda)^{-1}\| &= \left\| \gamma_{\lambda}(\alpha - \overline{B_{\lambda}})^{-1}\gamma_{\lambda}^* \right\| \\
 &\leq \|\gamma_{\lambda}\|^2 \left\| (\alpha - \overline{B_{\lambda}})^{-1} \right\| \\
 &\leq \frac{\|\gamma_{\lambda}\|^2}{\alpha - \nu_1(\lambda)}
 \end{aligned}$$

for all  $\alpha > \nu_1(\lambda)$ ; cf. Proposition 4.5 (ii). It follows that the right-hand side converges to 0 as  $\alpha \rightarrow +\infty$ . This proves assertion (ii).

To prove assertion (iii), let first  $\lambda = \lambda_0 \in \rho(-\Delta_{\Sigma, \alpha}) \cap (-\infty, 0)$  be fixed. Then

$$(-\Delta_{\Sigma, \alpha} - \lambda_0)^{-1} - (-\Delta_{\text{free}} - \lambda_0)^{-1} = \gamma_{\lambda_0}(\alpha - \overline{B_{\lambda_0}})^{-1}\gamma_{\lambda_0}^*. \tag{5.3}$$

Note that the identity (2.5) implies that  $\gamma_{\lambda_0}^*$  can also be regarded as a bounded operator from  $L^2(\mathbb{R}^3)$  to  $H^1(\Sigma)$  since the restriction map  $H^2(\mathbb{R}^3) \ni \varphi \mapsto \varphi|_{\Sigma} \in H^1(\Sigma)$  is continuous (cf., e.g., [13, Theorem 24.3]). In particular, it follows from the compactness of the embedding of  $H^1(\Sigma)$  into  $L^2(\Sigma)$  that  $\gamma_{\lambda_0}^*$  is compact. Since  $(\alpha - \overline{B_{\lambda_0}})^{-1}$  is a bounded operator in  $L^2(\Sigma)$ , the identity (5.3) implies that the resolvent difference in (3.2) is compact for  $\lambda = \lambda_0$ . For an arbitrary  $\lambda \in \rho(-\Delta_{\Sigma, \alpha}) \cap \rho(-\Delta_{\text{free}})$ , a simple calculation yields



$$\begin{aligned} & (-\Delta_{\Sigma,\alpha} - \lambda)^{-1} - (-\Delta_{\text{free}} - \lambda)^{-1} \\ &= U \left( (-\Delta_{\Sigma,\alpha} - \lambda_0)^{-1} - (-\Delta_{\text{free}} - \lambda_0)^{-1} \right) V, \end{aligned}$$

where

$$U = 1 + (\lambda - \lambda_0)(-\Delta_{\text{free}} - \lambda)^{-1} \quad \text{and} \quad V = 1 + (\lambda - \lambda_0)(-\Delta_{\Sigma,\alpha} - \lambda)^{-1}$$

are bounded operators in  $L^2(\mathbb{R}^3)$ . Now the claim follows from the assertion for  $\lambda_0$ . This proves (iii).

**5.2. Proof of Theorem 3.2**

It suffices to prove the assertion of Theorem 3.2 only for a fixed

$$\lambda = \lambda_0 \in \rho(-\Delta_{\Sigma,\alpha}) \cap (-\infty, 0).$$

Once it is established for  $\lambda_0$ , it follows for all  $\lambda \in \rho(-\Delta_{\Sigma,\alpha}) \cap \rho(-\Delta_{\text{free}})$  with an argument as in the proof of Theorem 3.1 (iii) and standard properties of singular values; cf. [38, II.§2.2]. When we denote by  $-\Delta_{\text{LB}}^\Sigma$  the Laplace–Beltrami operator in  $L^2(\Sigma)$  and write  $\Lambda := (I - \Delta_{\text{LB}}^\Sigma)^{1/2}$  then  $\Lambda$  is an isometric isomorphism between  $H^1(\Sigma)$  and  $L^2(\Sigma)$ . Moreover,  $\Lambda^{-1}$  is a compact, self-adjoint operator in  $L^2(\Sigma)$ , whose singular values satisfy  $s_k(\Lambda^{-1}) = O(1/k)$  as  $k \rightarrow +\infty$ ; cf. [2, (5.39) and the text below]. Since  $\gamma_{\lambda_0}^*$  is bounded from  $L^2(\mathbb{R}^3)$  to  $H^1(\Sigma)$  (see the proof of Theorem 3.1 (iii)) it follows that the operator  $\Lambda\gamma_{\lambda_0}^* : L^2(\mathbb{R}^3) \rightarrow L^2(\Sigma)$  is bounded and from

$$\gamma_{\lambda_0}^* = \Lambda^{-1}\Lambda\gamma_{\lambda_0}^*$$

we conclude  $s_k(\gamma_{\lambda_0}^*) = O(1/k)$  as  $k \rightarrow +\infty$ ; cf. [38, II.§2.2]. As a consequence, also  $\gamma_{\lambda_0} : L^2(\Sigma) \rightarrow L^2(\mathbb{R}^3)$  is a compact operator with  $s_k(\gamma_{\lambda_0}) = O(1/k)$  as  $k \rightarrow +\infty$ . Moreover, with the help of Corollary 2.2 in [38, Chapter II] we obtain

$$\begin{aligned} s_{3j-2}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1}\gamma_{\lambda_0}^*) &\leq s_{2j-1}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1})s_j(\gamma_{\lambda_0}^*) \\ &\leq s_j(\gamma_{\lambda_0})s_j((\alpha - \overline{B_\lambda})^{-1})s_j(\gamma_{\lambda_0}^*) \end{aligned} \tag{5.4}$$

for all  $j \in \mathbb{N}$ . Due to these observations and Proposition 4.5 (iii), there exists  $C = C(\lambda_0) > 0$  such that

$$s_j(\gamma_{\lambda_0}) \leq \frac{C}{j}, \quad s_j((\alpha - \overline{B_\lambda})^{-1}) \leq \frac{C}{\ln j}, \quad \text{and} \quad s_j(\gamma_{\lambda_0}^*) \leq \frac{C}{j}$$

hold for all  $j \in \mathbb{N}$ . From this the claim of the theorem follows for  $\lambda = \lambda_0$ . Indeed, for  $j \geq 2$ , with the help of (5.4) we get

$$s_{3j-2}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1}\gamma_{\lambda_0}^*) \leq \frac{C^3}{j^2 \ln j} \leq \frac{27C^3}{(3j)^2 \ln(3j)}$$

since  $\ln j = \frac{1}{3} \ln(j^3) \geq \frac{1}{3} \ln(3j)$ . As

$$\begin{aligned} s_{3j}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1}\gamma_{\lambda_0}^*) &\leq s_{3j-1}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1}\gamma_{\lambda_0}^*) \\ &\leq s_{3j-2}(\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1}\gamma_{\lambda_0}^*) \end{aligned}$$

and

$$\frac{27C^3}{(3j)^2 \ln(3j)} \leq \frac{27C^3}{(3j-1)^2 \ln(3j-1)} \leq \frac{27C^3}{(3j-2)^2 \ln(3j-2)}$$

we observe

$$s_k (\gamma_{\lambda_0}(\alpha - \overline{B_\lambda})^{-1} \gamma_{\lambda_0}^*) \leq \frac{27C^3}{k^2 \ln k}$$

for all  $k \in \mathbb{N}$ ,  $k \geq 4$ . This yields the assertion of the theorem.

**5.3. Proof of Theorem 3.3 and Corollary 3.4**

Let us first prove Theorem 3.3. For  $\lambda \leq 0$ , let us denote by  $\nu_j(\lambda)$  the eigenvalues of the operator  $\overline{B_\lambda}$ , ordered nonincreasingly and counted with multiplicities; cf. Proposition 4.5 (iii). We remark that by Theorem 3.1 (i) and Proposition 4.5 (iv) the number  $N_\alpha$  of negative eigenvalues of  $-\Delta_{\Sigma, \alpha}$  counted with multiplicities coincides with the number of eigenvalues of  $\overline{B_0}$  larger than  $\alpha$ , counted with multiplicities. Moreover, let  $\mathcal{T}$  be a circle of radius  $R = \frac{L}{2\pi}$ , where  $L$  is the length of  $\Sigma$ . We denote by  $B_\lambda^\mathcal{T}$  the analog of  $B_\lambda$  where  $\Sigma$  is replaced by the circle  $\mathcal{T}$ , and by  $\nu_j^\mathcal{T}(\lambda)$  the eigenvalues of its closure. From (4.18) with  $\lambda = 0$ , it follows with the min-max principle that

$$\nu_j^\mathcal{T}(0) - \|D_0\| \leq \nu_j(0) \leq \nu_j^\mathcal{T}(0) + \|D_0\|, \quad j = 1, 2, \dots$$

Taking into account (4.17), we obtain

$$\nu_j^\mathcal{T}(0) - d_\Sigma \leq \nu_j(0) \leq \nu_j^\mathcal{T}(0) + d_\Sigma, \quad j = 1, 2, \dots \tag{5.5}$$

Assume first that  $\alpha - d_\Sigma \geq \frac{\ln(4R)}{2\pi}$ . For  $\lambda < 0$  and  $j = 1, 2, \dots$ , we obtain from Proposition 4.5 (iv), (5.5), and Lemma 4.2 (ii)

$$\nu_j(\lambda) < \nu_j(0) \leq \nu_1(0) \leq \nu_1^\mathcal{T}(0) + d_\Sigma = \frac{\ln(4R)}{2\pi} + d_\Sigma \leq \alpha.$$

In particular,  $\alpha \notin \sigma_p(\overline{B_\lambda})$  for all  $\lambda < 0$ . From this and Theorem 3.1 (i), it follows  $\lambda \notin \sigma_p(-\Delta_{\Sigma, \alpha})$  for all  $\lambda < 0$ , hence  $N_\alpha = 0$ .

Assume now  $\alpha + d_\Sigma \in I_r$  for some  $r \geq 0$  and  $\alpha - d_\Sigma \in I_l$  for some  $l \geq 0$ . By means of Lemma 4.2 (ii), this implies

$$\nu_{2r+2}^\mathcal{T}(0) \leq \alpha + d_\Sigma < \nu_{2r+1}^\mathcal{T}(0) \tag{5.6}$$

and

$$\nu_{2l+2}^\mathcal{T}(0) \leq \alpha - d_\Sigma < \nu_{2l+1}^\mathcal{T}(0). \tag{5.7}$$

From (5.6), (5.7) and (5.5), it follows

$$\nu_{2l+2}(0) \leq \nu_{2l+2}^\mathcal{T}(0) + d_\Sigma \leq \alpha < \nu_{2r+1}^\mathcal{T}(0) - d_\Sigma \leq \nu_{2r+1}(0). \tag{5.8}$$

Due to Proposition 4.5 (iv), the functions  $\lambda \mapsto \nu_j(\lambda)$  are continuous and strictly increasing and satisfy  $\nu_j(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ ,  $j = 1, 2, \dots$ . Thus, by (5.8) for each  $j \leq 2r+1$  there exists precisely one  $\lambda_j < 0$  such that  $\nu_j(\lambda_j) = \alpha$ . From Theorem 3.1 (i), we conclude that each such  $\lambda_j$  is an eigenvalue of  $-\Delta_{\Sigma, \alpha}$  and hence we obtain the estimate

$$2r + 1 \leq N_\alpha.$$

In the same way, (5.8) implies that for any  $j \geq 2l + 2$  there exists no  $\lambda < 0$  such that  $\nu_j(\lambda) = \alpha$  and that for each  $j \in \{k : 2r + 2 \leq k \leq 2l + 1\}$  there exists at most one  $\lambda_j < 0$  such that  $\nu_j(\lambda_j) = \alpha$ . Theorem 3.1 (i) yields that each such  $\lambda_j$  is an eigenvalue of  $-\Delta_{\Sigma, \alpha}$  and, therefore,

$$N_\alpha \leq 2l + 1.$$

In the remaining case,  $\alpha + d_\Sigma \in I_r$  with  $r = -1$  it is clear that

$$2r + 1 = -1 \leq N_\alpha,$$

and the upper estimate for  $N_\alpha$  follows as above. This completes the proof of the theorem.

Let us now turn to the proof of the corollary. As in Theorem 3.3, let  $r$  and  $l$  such that  $\alpha + d_\Sigma \in I_r$  and  $\alpha - d_\Sigma \in I_l$ . The condition  $\alpha + d_\Sigma < \frac{\ln(4R)}{2\pi} - \frac{1}{\pi}$  ensures  $1 \leq r \leq l$ . The proof is based on the estimates

$$\ln k + \gamma + \frac{1}{2k} - \frac{1}{12k^2} < H_k < \ln k + \gamma + \frac{1}{2k} - \frac{1}{12k^2} + \frac{1}{120k^4} \tag{5.9}$$

for the harmonic sum  $H_k = \sum_{j=1}^k \frac{1}{j}$ ,  $k \geq 1$ , see e.g. [40, (9.89)]. Since  $\sum_{j=1}^k \frac{1}{2j-1} = H_{2k} - \frac{1}{2}H_k$ , it follows from (5.9)

$$\begin{aligned} \sum_{j=1}^k \frac{1}{2j-1} &> \ln(2k) + \gamma + \frac{1}{4k} - \frac{1}{48k^2} - \frac{1}{2} \left( \ln k + \gamma + \frac{1}{2k} - \frac{1}{12k^2} + \frac{1}{120k^4} \right) \\ &= \frac{\ln k + \ln 4 + \gamma}{2} + \frac{1}{48k^2} - \frac{1}{240k^4} \\ &> \frac{\ln k + \ln 4 + \gamma}{2}. \end{aligned}$$

Hence,  $\alpha - d_\Sigma \in I_l$  implies

$$\alpha - d_\Sigma < \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^l \frac{1}{2j-1} < \frac{\ln(4R)}{2\pi} - \frac{\ln l + \ln 4 + \gamma}{2\pi}$$

and, therefore,

$$\ln l < -2\pi(\alpha - d_\Sigma) + \ln R - \gamma. \tag{5.10}$$

Using  $N_\alpha \leq 2l + 1$  from Theorem 3.3 and the estimate (5.10), we get

$$N_\alpha - 2Re^{-2\pi(\alpha - d_\Sigma) - \gamma} \leq 2l + 1 - 2e^{-2\pi(\alpha - d_\Sigma) + \ln R - \gamma} < 2l + 1 - 2e^{\ln l} = 1$$

which yields the upper estimate for  $N_\alpha$  in (3.4).

For the lower estimate in (3.4), we deduce from (5.9) the estimate

$$\begin{aligned} & \sum_{j=1}^k \frac{1}{2j-1} \\ & < \ln(2k) + \gamma + \frac{1}{4k} - \frac{1}{48k^2} + \frac{1}{1920k^4} - \frac{1}{2} \left( \ln k + \gamma + \frac{1}{2k} - \frac{1}{12k^2} \right) \\ & = \frac{\ln k + \ln 4 + \gamma}{2} + \frac{1}{48k^2} + \frac{1}{1920k^4} \\ & < \frac{\ln k + \ln 4 + \gamma + \frac{1}{23k^2}}{2}. \end{aligned}$$

Hence,  $\alpha + d_\Sigma \in I_r$  implies

$$\begin{aligned} \alpha + d_\Sigma & \geq \frac{\ln(4R)}{2\pi} - \frac{1}{\pi} \sum_{j=1}^{r+1} \frac{1}{2j-1} \\ & > \frac{\ln(4R)}{2\pi} - \frac{\ln(r+1) + \ln 4 + \gamma + \frac{1}{23(r+1)^2}}{2\pi} \end{aligned}$$

and, therefore,

$$\ln(r+1) + \frac{1}{23(r+1)^2} > -2\pi(\alpha + d_\Sigma) + \ln R - \gamma. \tag{5.11}$$

Using  $N_\alpha \geq 2r + 1$  from Theorem 3.3 and the estimate (5.11), we get

$$\begin{aligned} N_\alpha - 2Re^{-2\pi(\alpha+d_\Sigma)-\gamma} & \geq 2r + 1 - 2e^{-2\pi(\alpha+d_\Sigma)+\ln R-\gamma} \\ & > 2r + 1 - 2e^{\ln(r+1)+\frac{1}{23(r+1)^2}} \\ & = 2(r+1) - 1 - 2(r+1)e^{\frac{1}{23(r+1)^2}} \\ & = 2(r+1) \left( 1 - e^{\frac{1}{23(r+1)^2}} \right) - 1 =: g(r). \end{aligned}$$

As  $g'(r) > 0$  for all  $r \geq 1$ , the minimum of  $g$  for  $r \geq 1$  is attained at  $r = 1$ . Hence,

$$N_\alpha - 2Re^{-2\pi(\alpha+d_\Sigma)-\gamma} > 4 \left( 1 - e^{\frac{1}{92}} \right) - 1,$$

which gives the lower estimate in (3.4).

**5.4. Proof of Theorem 3.6**

The proof of Theorem 3.6 follows the ideas of [25, 28]. Suppose that  $\Sigma$  is not a circle. Then the strict inequality

$$\int_0^L |\sigma(s+u) - \sigma(s)| ds < \frac{L^2}{\pi} \sin \frac{\pi u}{L}, \quad u \in (0, L), \tag{5.12}$$

holds, where  $\sigma$  is identified with its  $L$ -periodic extension to all of  $\mathbb{R}$ . For  $u \in (0, \frac{L}{2}]$ , the inequality (5.12) follows from [28, Theorem 2.2 and Proposition 2.1]. As every  $u \in (\frac{L}{2}, L)$  can be written as  $u = L - v$  with  $v \in (0, \frac{L}{2})$ ,

the substitution  $t = s - v$  and the periodicity of  $\sigma$  yield for  $u \in (\frac{L}{2}, L)$

$$\begin{aligned} \int_0^L |\sigma(s + u) - \sigma(s)| \, ds &= \int_0^L |\sigma(s - v) - \sigma(s)| \, ds \\ &= \int_0^L |\sigma(t) - \sigma(t + v)| \, dt \\ &< \frac{L^2}{\pi} \sin \frac{\pi v}{L} \\ &= \frac{L^2}{\pi} \sin \frac{\pi u}{L}, \end{aligned}$$

i.e., the estimate (5.12) holds for all  $u \in (0, L)$ .

In the following, denote by  $\lambda_1 = \min \sigma(-\Delta_{\mathcal{T}, \alpha}) < 0$  the smallest eigenvalue of  $-\Delta_{\mathcal{T}, \alpha}$  (cf. Corollary 3.5) and let  $\nu_1^{\mathcal{T}}(\lambda_1)$  be the largest eigenvalue of  $\overline{B_{\lambda_1}^{\mathcal{T}}}$ . By Theorem 3.1 (i), we have  $\alpha \in \sigma_p(\overline{B_{\lambda_1}^{\mathcal{T}}})$  and, in particular,  $\alpha \leq \nu_1^{\mathcal{T}}(\lambda_1)$ .

We claim that

$$\nu_1^{\mathcal{T}}(\lambda_1) < \nu_1(\lambda_1) \tag{5.13}$$

holds. To see this, note first that (4.18) implies

$$\overline{B_{\lambda_1}} = D_{\lambda_1} + J^* \overline{B_{\lambda_1}^{\mathcal{T}}} J, \tag{5.14}$$

where  $J : L^2(\Sigma) \rightarrow L^2(\mathcal{T})$  is the unitary mapping given in (4.16) and the compact operator  $D_{\lambda_1}$  in  $L^2(\Sigma)$  is given by

$$(D_{\lambda_1} h)(\sigma(t)) = \int_0^L h(\sigma(s)) \left[ \frac{e^{-\sqrt{-\lambda_1}|\sigma(t)-\sigma(s)|}}{4\pi|\sigma(t)-\sigma(s)|} - \frac{e^{-\sqrt{-\lambda_1}|\tau(t)-\tau(s)|}}{4\pi|\tau(t)-\tau(s)|} \right] ds$$

for  $h \in L^2(\Sigma)$ . It follows from Lemma 4.3 (iv) and (5.14) that for the constant function  $h = \frac{1}{\sqrt{L}}$  on  $\Sigma$  (which implies  $\|h\|_{L^2(\Sigma)} = 1$ ) we have

$$\begin{aligned} \langle \overline{B_{\lambda_1}} h, h \rangle_{L^2(\Sigma)} &= \langle D_{\lambda_1} h, h \rangle_{L^2(\Sigma)} + \left\langle \overline{B_{\lambda_1}^{\mathcal{T}}} Jh, Jh \right\rangle_{L^2(\mathcal{T})} \\ &= \langle D_{\lambda_1} h, h \rangle_{L^2(\Sigma)} + \nu_1^{\mathcal{T}}(\lambda_1). \end{aligned} \tag{5.15}$$

Our aim is to estimate the term  $\langle D_{\lambda_1} h, h \rangle_{L^2(\Sigma)}$ . For this purpose, we define the function

$$G(x) = \frac{e^{-\sqrt{-\lambda_1}x}}{4\pi x}, \quad x > 0.$$

It is easy to see that  $G$  is strictly monotone decreasing and convex. Hence, (5.12) and the monotonicity of  $G$  imply

$$G\left(\frac{L}{\pi} \sin \frac{\pi u}{L}\right) < G\left(\frac{1}{L} \int_0^L |\sigma(s + u) - \sigma(s)| ds\right) \tag{5.16}$$

for each  $u \in (0, L)$ . Using Jensen’s inequality, see e.g. [56, Theorem 3.3], the convexity of  $G$  implies

$$G\left(\frac{1}{L} \int_0^L |\sigma(s + u) - \sigma(s)| ds\right) \leq \frac{1}{L} \int_0^L G(|\sigma(s + u) - \sigma(s)|) ds. \tag{5.17}$$

Combining (5.16) and (5.17), we observe

$$\begin{aligned}
 0 &< \int_0^L \left( \int_0^L G(|\sigma(s+u) - \sigma(s)|) \, ds - LG \left( \frac{L}{\pi} \sin \frac{\pi u}{L} \right) \right) du \\
 &= \int_0^L \int_0^L G(|\sigma(s+u) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi u}{L} \right) \, dud s. \tag{5.18}
 \end{aligned}$$

Moreover, for each  $s \in (0, L)$  with the substitution  $t = s + u$ , we get

$$\begin{aligned}
 &\int_0^L G(|\sigma(s+u) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi u}{L} \right) \, du \\
 &= \int_s^{L+s} G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi(t-s)}{L} \right) \, dt \\
 &= \int_s^L G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi(t-s)}{L} \right) \, dt \\
 &\quad + \int_0^s G(|\sigma(t+L) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi(t+L-s)}{L} \right) \, dt \\
 &= \int_s^L G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi(t-s)}{L} \right) \, dt \\
 &\quad + \int_0^s G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi(s-t)}{L} \right) \, dt \\
 &= \int_0^L G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi|t-s|}{L} \right) \, dt.
 \end{aligned}$$

Therefore, (5.18) can be rewritten as

$$0 < \int_0^L \int_0^L G(|\sigma(t) - \sigma(s)|) - G \left( \frac{L}{\pi} \sin \frac{\pi|t-s|}{L} \right) \, dt ds.$$

From the last equality and (4.1) (with  $\sigma$  replaced by  $\tau$ ), we conclude

$$\begin{aligned}
 \langle D_{\lambda_1} h, h \rangle_{L^2(\Sigma)} &= \frac{1}{L} \int_0^L \int_0^L \frac{e^{-\sqrt{-\lambda_1}|\sigma(t)-\sigma(s)|}}{4\pi|\sigma(t) - \sigma(s)|} - \frac{e^{-\sqrt{-\lambda_1}|\tau(t)-\tau(s)|}}{4\pi|\tau(t) - \tau(s)|} \, ds dt \\
 &> 0
 \end{aligned}$$

for the constant function  $h = \frac{1}{\sqrt{L}}$ . Hence, (5.15) leads to

$$\langle \overline{B}_{\lambda_1} h, h \rangle_{L^2(\Sigma)} > \nu_1^T(\lambda_1)$$

for the constant function  $h = \frac{1}{\sqrt{L}}$  and hence (5.13) follows. In particular,

$$\alpha \leq \nu_1^T(\lambda_1) < \nu_1(\lambda_1).$$

As the function  $\lambda \mapsto \nu_1(\lambda)$  is continuous and strictly increasing on  $(-\infty, 0]$  by Proposition 4.5 (iv) and  $\nu_1(\lambda) \rightarrow -\infty$  as  $\lambda \rightarrow -\infty$ , there exists  $\lambda_2 < \lambda_1$  such that  $\alpha = \nu_1(\lambda_2)$ . By Theorem 3.1 (i),  $\lambda_2$  is an eigenvalue of  $-\Delta_{\Sigma, \alpha}$ . Thus,

$$\min \sigma(-\Delta_{\Sigma, \alpha}) \leq \lambda_2 < \lambda_1 = \min \sigma(-\Delta_{\mathcal{T}, \alpha}),$$

which completes the proof of Theorem 3.6.

**5.5. Proof of Theorem 3.8**

Consider the scattering pair  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma, \alpha}\}$  with  $\alpha \in \mathbb{R} \setminus \{0\}$  and fix  $\eta < 0$  such that  $0 \in \rho(\overline{B_\eta} - \alpha)$ , which is possible according to Proposition 4.5 (ii) and (iv). As in (A.9) and (A.10), consider the symmetric operator

$$Su = -\Delta u, \quad \text{dom } S = \{u \in H^2(\mathbb{R}^3) : u|_\Sigma = 0\},$$

and the operator

$$Tu = -\Delta u - h\delta_\Sigma, \quad \text{dom } T = H^2(\mathbb{R}^3) \dot{+} \{\gamma_\eta h : h \in \text{dom } \overline{B_\eta}\},$$

where  $\gamma_\eta h = (-\Delta - \eta)^{-1}(h\delta_\Sigma)$  is as in (2.3). Then  $\overline{T} = S^*$  according to Proposition A.5. Now we slightly modify the boundary maps in Proposition A.5 such that Theorem A.4 can be applied directly to the pair  $\{-\Delta_{\text{free}}, -\Delta_{\Sigma, \alpha}\}$ . More precisely, we claim that  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$ , where

$$\Gamma_0 u = h \quad \text{and} \quad \Gamma_1 u = u_c|_\Sigma + (\overline{B_\eta} - \alpha)h, \quad u = u_c + \gamma_\eta h \in \text{dom } T, \quad (5.19)$$

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

$$-\Delta_{\text{free}} = T \upharpoonright \ker \Gamma_0 \quad \text{and} \quad -\Delta_{\Sigma, \alpha} = T \upharpoonright \ker \Gamma_1. \quad (5.20)$$

The  $\gamma$ -field and Weyl function corresponding to  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  are given by

$$\gamma(\lambda)h = (-\Delta - \lambda)^{-1}(h\delta_\Sigma) \quad \text{and} \quad M(\lambda)h = N(\lambda)h + (\overline{B_\eta} - \alpha)h, \quad (5.21)$$

where  $\lambda \in \mathbb{C} \setminus [0, \infty)$ ,  $h \in \text{dom } \overline{B_\eta}$ , and the function  $N$  is as in (3.5).

In fact, the identities in (5.20) hold by construction and Proposition A.5. To verify the abstract Green identity for the boundary maps in (5.19), recall from (A.17) in the proof of Proposition A.5 that for  $u, v \in \text{dom } T$  such that  $u = u_c + \gamma_\eta h$  and  $v = v_c + \gamma_\eta k$  the identity

$$\langle Tu, v \rangle_{L^2(\mathbb{R}^3)} - \langle u, Tv \rangle_{L^2(\mathbb{R}^3)} = \langle u_c|_\Sigma, k \rangle_{L^2(\Sigma)} - \langle h, v_c|_\Sigma \rangle_{L^2(\Sigma)}$$

holds. Since  $(\overline{B_\eta} - \alpha)$  is a self-adjoint operator in  $L^2(\Sigma)$ , we have

$$\begin{aligned} & \langle u_c|_\Sigma, k \rangle_{L^2(\Sigma)} - \langle h, v_c|_\Sigma \rangle_{L^2(\Sigma)} \\ &= \langle u_c|_\Sigma + (\overline{B_\eta} - \alpha)h, k \rangle_{L^2(\Sigma)} - \langle h, v_c|_\Sigma + (\overline{B_\eta} - \alpha)k \rangle_{L^2(\Sigma)} \\ &= \langle \Gamma_1 u, \Gamma_0 v \rangle_{L^2(\Sigma)} - \langle \Gamma_0 u, \Gamma_1 v \rangle_{L^2(\Sigma)} \end{aligned}$$

and hence the Green identity is valid. The same argument as in the proof of Proposition A.5 shows that the range of the mapping  $u \mapsto (\Gamma_0 u, \Gamma_1 u)^\top$  is dense in  $L^2(\Sigma) \times L^2(\Sigma)$ . Hence,  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  is a quasi boundary triple for  $S^*$ . Since  $\Gamma_0$  is the same map as in Proposition A.5, the corresponding  $\gamma$ -field has the same form as in Proposition A.5. The form of the Weyl function in (5.21) follows from

$$M(\eta)h = \Gamma_1 \gamma(\eta)h = \Gamma_1 (-\Delta - \eta)^{-1}(h\delta_\Sigma) = (\overline{B_\eta} - \alpha)h$$

for  $h \in \text{ran } \Gamma_0 = \text{dom } \overline{B_\eta}$  and (3.5) in the same way as in the proof of Proposition A.5; cf. (4.26), (4.28), and Remark A.6.

Now we complete the proof of Theorem 3.8. Consider the quasi boundary triple  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  in (5.19). It follows from (5.21), (2.3) and the proof of Theorem 3.2 that

$$\overline{\gamma(\eta)} = \gamma_\eta \in \mathfrak{S}_2(L^2(\Sigma), L^2(\mathbb{R}^3)). \quad (5.22)$$

Moreover, since  $\eta < 0$  was chosen such that  $0 \in \rho(\overline{B_\eta} - \alpha)$  it is clear that the operator  $M(\eta)^{-1} = (\overline{B_\eta} - \alpha)^{-1}$  is bounded in  $L^2(\Sigma)$ . Note also that

$$\overline{\text{Im } M(\lambda)} = \text{Im } N(\lambda), \quad \lambda \in \mathbb{C} \setminus [0, \infty),$$

holds by (5.21). Hence, the assumptions in Theorem A.4 are satisfied and the assertions (i), (iii), and (iv) in Theorem 3.8 follow. Observe that by (5.21) and (A.4)

$$\begin{aligned} N(\lambda) &= (\lambda - \eta)\gamma(\eta)^*(-\Delta_{\text{free}} - \eta)(-\Delta_{\text{free}} - \lambda)^{-1}\overline{\gamma(\eta)} \\ &= (\lambda - \eta)\gamma(\eta)^*\overline{\gamma(\eta)} + (\lambda - \eta)^2\gamma(\eta)^*(-\Delta_{\text{free}} - \lambda)^{-1}\overline{\gamma(\eta)} \end{aligned}$$

holds for  $\lambda \in \mathbb{C} \setminus [0, \infty)$ . Therefore, (5.22) and [6, Proposition 3.14] yield that the limit  $N(\lambda + i0)$  exists in the Hilbert–Schmidt norm for a.e.  $\lambda \in [0, \infty)$ , that is, assertion (ii) in Theorem 3.8 holds. This completes the proof.

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### Appendix A. Quasi Boundary Triples and Their Weyl Functions

In this appendix, we briefly review the abstract notions of quasi boundary triples and their Weyl functions from extension theory of symmetric operators in Hilbert spaces, and relate them to the Schrödinger operators  $-\Delta_{\text{free}}$  and  $-\Delta_{\Sigma, \alpha}$ . Furthermore, we recall a representation formula for the scattering matrix in terms of the Weyl function of a quasi boundary triple from [10], which is the main ingredient in the proof of Theorem 3.8. For more details on quasi boundary triples and their Weyl functions, we refer the reader to [7, 8], and for generalized and ordinary boundary triples to [20, 23, 24].



**Definition A.1.** Let  $S$  be a densely defined, closed, symmetric operator in a Hilbert space  $(\mathfrak{H}, \langle \cdot, \cdot \rangle_{\mathfrak{H}})$  and assume that  $T$  is a linear operator in  $\mathfrak{H}$  such that  $\overline{T} = S^*$ . A triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is a *quasi boundary triple* for  $S^*$  if  $(\mathcal{G}, \langle \cdot, \cdot \rangle_{\mathcal{G}})$  is a Hilbert space and  $\Gamma_0, \Gamma_1 : \text{dom } T \rightarrow \mathcal{G}$  are linear mappings such that the following holds.

(i) For all  $u, v \in \text{dom } T$ , one has

$$\langle Tu, v \rangle_{\mathfrak{H}} - \langle u, Tv \rangle_{\mathfrak{H}} = \langle \Gamma_1 u, \Gamma_0 v \rangle_{\mathcal{G}} - \langle \Gamma_0 u, \Gamma_1 v \rangle_{\mathcal{G}}.$$

(ii) The range of the mapping  $(\Gamma_0, \Gamma_1)^{\top} : \text{dom } T \rightarrow \mathcal{G} \times \mathcal{G}$  is dense.

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

If  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is a quasi boundary triple for  $\overline{T} = S^*$ , then

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

Moreover, if  $\text{ran } \Gamma_0 = \mathcal{G}$ , then  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is a generalized boundary triple in the sense of [24, Section 6], and if  $\text{ran}(\Gamma_0, \Gamma_1)^{\top} = \mathcal{G} \times \mathcal{G}$  then  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is an ordinary boundary triple; cf. [20, 23]. In the latter case, it follows that  $T = S^*$  and hence the abstract Green identity in Definition A.1 (i) holds for all  $u, v \in \text{dom } S^*$ . We remark that for an ordinary boundary triple, condition (iii) in Definition A.1 is automatically satisfied.

A quasi boundary triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  for  $\overline{T} = S^*$  is a useful tool to describe the extensions of  $S$  which are contained in  $T$  via abstract boundary conditions in the auxiliary Hilbert space  $\mathcal{G}$ . However, in this context it is important to note that not all self-adjoint extensions of  $S$  in  $\mathfrak{H}$  are covered, but only those which are also restrictions of  $T$ . Furthermore, a self-adjoint parameter  $\Theta$  in  $\mathcal{G}$  does not automatically lead to a self-adjoint extension via

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

as one is used to from the theory of ordinary boundary triples. In general,  $A_{\Theta}$  in (A.1) is only symmetric in  $\mathfrak{H}$ , not necessarily closed, and one has to impose additional conditions on  $\Theta$  or on other involved objects to ensure self-adjointness of the extension  $A_{\Theta}$ , see, e.g., [7, 8].

Next we recall [8, Theorem 6.11] which is very useful for the construction of quasi boundary triples and provides a method to determine the adjoint of a symmetric operator.

**Theorem A.2.** *Let  $T$  be a linear operator in a Hilbert space  $(\mathfrak{H}, \langle \cdot, \cdot \rangle_{\mathfrak{H}})$ , let  $(\mathcal{G}, \langle \cdot, \cdot \rangle_{\mathcal{G}})$  be a Hilbert space, and assume that  $\Gamma_0, \Gamma_1 : \text{dom } T \rightarrow \mathcal{G}$  are linear mappings such that the following holds.*

(i) *For all  $u, v \in \text{dom } T$ , one has*

$$\langle Tu, v \rangle_{\mathfrak{H}} - \langle u, Tv \rangle_{\mathfrak{H}} = \langle \Gamma_1 u, \Gamma_0 v \rangle_{\mathcal{G}} - \langle \Gamma_0 u, \Gamma_1 v \rangle_{\mathcal{G}}.$$

(ii)  *$\text{ran}(\Gamma_0, \Gamma_1)^{\top}$  is dense in  $\mathcal{G} \times \mathcal{G}$  and  $\ker \Gamma_0 \cap \ker \Gamma_1$  is dense in  $\mathfrak{H}$ .*

(iii) *There exists a self-adjoint operator  $A_0$  in  $\mathfrak{H}$  such that  $A_0 \subset T \upharpoonright \ker \Gamma_0$ .*

*Then  $S := T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1)$  is a densely defined, closed, symmetric operator in  $\mathfrak{H}$  such that  $\overline{T} = S^*$ , 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 notion of the  $\gamma$ -field and Weyl function associated with a quasi boundary triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  for  $\bar{T} = S^*$ . First of all it follows from the direct sum decomposition  $\text{dom } T = \text{dom } A_0 \dot{+} \ker(T - \lambda)$ ,  $\lambda \in \rho(A_0)$ , and  $\text{dom } A_0 = \ker \Gamma_0$  that the restriction of the boundary map  $\Gamma_0$  onto  $\ker(T - \lambda)$  is invertible. The inverse

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

is a densely defined operator from  $\mathcal{G}$  into  $\mathfrak{H}$ . The function  $\lambda \mapsto \gamma(\lambda)$  is called the  $\gamma$ -field associated to  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ . The Weyl function  $M$  associated to  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is defined by

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

The values  $M(\lambda)$  of the Weyl function are densely defined operators in  $\mathcal{G}$ , which may be unbounded and not closed in general. If one views the boundary maps  $\Gamma_0$  and  $\Gamma_1$  as abstract Dirichlet and Neumann trace maps then the values of the Weyl function can be interpreted as abstract analogs of the Dirichlet-to-Neumann map in the theory of elliptic PDEs. For  $\lambda, \mu \in \rho(A_0)$  and  $h \in \text{ran } \Gamma_0$ , we note the useful identities

$$\gamma(\lambda)^* = \Gamma_1(A_0 - \bar{\lambda})^{-1} \tag{A.2}$$

and

$$\gamma(\lambda)h = (A_0 - \mu)(A_0 - \lambda)^{-1}\gamma(\mu)h \tag{A.3}$$

as well as

$$M(\lambda)h = M(\mu)^*h + (\lambda - \mu)\gamma(\mu)^*(A_0 - \mu)(A_0 - \lambda)^{-1}\gamma(\mu)h \tag{A.4}$$

for the  $\gamma$ -field and Weyl function, and refer the reader for more details and proofs of the above identities to [7, 8].

The following theorem from [7, 8] contains a Krein-type resolvent formula and provides a criterion to show self-adjointness of the extension  $A_\Theta$  in (A.1).

**Theorem A.3.** *Let  $S$  be a densely defined, closed, symmetric operator in a Hilbert space  $(\mathfrak{H}, \langle \cdot, \cdot \rangle_{\mathfrak{H}})$  and let  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  be a quasi boundary triple for  $\bar{T} = S^*$  with  $A_0 = T \upharpoonright \ker \Gamma_0$  and  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Let  $\Theta$  be an operator in  $\mathcal{G}$  and let*

$$A_\Theta = T \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0).$$

*Assume, in addition, that  $\lambda \in \rho(A_0)$  is not an eigenvalue of  $A_\Theta$  or, equivalently,  $\ker(\Theta - M(\lambda)) = \{0\}$ . Then the following assertions hold.*

- (i)  *$u \in \text{ran}(A_\Theta - \lambda)$  if and only if  $\gamma(\bar{\lambda})^*u \in \text{dom}(\Theta - M(\lambda))^{-1}$ .*
- (ii) *For all  $u \in \text{ran}(A_\Theta - \lambda)$  one has*

$$(A_\Theta - \lambda)^{-1}u = (A_0 - \lambda)^{-1}u + \gamma(\lambda) (\Theta - M(\lambda))^{-1} \gamma(\bar{\lambda})^*u. \tag{A.5}$$

*In particular, if  $\Theta$  is a symmetric operator in  $\mathcal{G}$  and  $\text{ran } \gamma(\bar{\lambda})^*$  is contained in  $\text{dom}(\Theta - M(\lambda))^{-1}$  for some  $\lambda \in \mathbb{C}^+$  and some  $\lambda \in \mathbb{C}^-$  then  $A_\Theta$  is self-adjoint in  $\mathfrak{H}$  and the resolvent formula (A.5) holds for all  $\lambda \in \rho(A_\Theta) \cap \rho(A_0)$  and all  $u \in \mathfrak{H}$ .*

Next, we provide a slightly generalized variant of the representation formula for the scattering matrix from [10]. Let again  $S$  be a densely defined, closed, symmetric operator in a Hilbert space  $(\mathfrak{H}, \langle \cdot, \cdot \rangle_{\mathfrak{H}})$  and let  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  be a quasi boundary triple for  $\bar{T} = S^*$  with  $A_0 = T \upharpoonright \ker \Gamma_0$  and  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Assume, in addition, that the extension

$$A_1 = T \upharpoonright \ker \Gamma_1$$

is self-adjoint in  $\mathfrak{H}$ ; in general  $A_1$  is only symmetric in  $\mathfrak{H}$  and not necessarily closed. Denote the absolutely continuous subspaces of  $A_0$  and  $A_1$  by  $\mathfrak{H}^{\text{ac}}(A_0)$  and  $\mathfrak{H}^{\text{ac}}(A_1)$ , respectively, let  $P^{\text{ac}}(A_0)$  be the orthogonal projection onto  $\mathfrak{H}^{\text{ac}}(A_0)$  and let

$$A_0^{\text{ac}} = A_0 \upharpoonright (\text{dom } A_0 \cap \mathfrak{H}^{\text{ac}}(A_0))$$

in  $\mathfrak{H}^{\text{ac}}(A_0)$  be the absolutely continuous part of  $A_0$ . If the difference of the resolvents of  $A_0$  and  $A_1$  is a trace class operator, that is,

$$(A_1 - \lambda)^{-1} - (A_0 - \lambda)^{-1} \in \mathfrak{S}_1(\mathfrak{H}) \tag{A.6}$$

for some, and hence for all,  $\lambda \in \rho(A_0) \cap \rho(A_1)$  then the wave operators

$$W_{\pm}(A_0, A_1) := s - \lim_{t \rightarrow \pm\infty} e^{itA_1} e^{-itA_0} P^{\text{ac}}(A_0)$$

exist and satisfy  $\text{ran } W_{\pm}(A_0, A_1) = \mathfrak{H}^{\text{ac}}(A_1)$  according to the Birman–Krein theorem [14]. It follows that the scattering operator

$$S(A_0, A_1) := W_+(A_0, A_1)^* W_-(A_0, A_1)$$

is unitary in the absolutely continuous subspace  $\mathfrak{H}^{\text{ac}}(A_0)$  of  $A_0$ , and that  $S(A_0, A_1)$  is unitarily equivalent to a multiplication operator  $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$  in a spectral representation of the absolutely continuous part  $A_0^{\text{ac}}$  of  $A_0$ . The family  $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$  is called the *scattering matrix* of the pair  $\{A_0, A_1\}$ ; cf. [6, 42, 55, 61].

In general, the underlying closed symmetric operator  $S$  is not simple (or completely non-self-adjoint) and hence its self-adjoint part is reflected in the scattering matrix of  $\{A_0, A_1\}$ . More precisely, if  $S$  is not simple then there is a nontrivial orthogonal decomposition of the Hilbert space  $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$  such that

$$S = S_1 \oplus S_2, \tag{A.7}$$

where  $S_1$  is a simple symmetric operator in  $\mathfrak{H}_1$  and  $S_2$  is a self-adjoint operator in  $\mathfrak{H}_2$ . Since  $A_0$  and  $A_1$  are self-adjoint extensions of  $S$ , there exist self-adjoint extensions  $B_0$  and  $B_1$  of  $S_1$  in  $\mathfrak{H}_1$  such that

$$A_0 = B_0 \oplus S_2 \quad \text{and} \quad A_1 = B_1 \oplus S_2. \tag{A.8}$$

In the following, let  $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{\lambda})$  be a spectral representation of the absolutely continuous part  $S_2^{\text{ac}}$  of the self-adjoint operator  $S_2$  in  $\mathfrak{H}_2$ .

Now we can formulate a variant of [10, Theorem 3.1 and Corollary 3.3] which is suitable for our purposes. Instead of generalized boundary triples, the result is stated for quasi boundary triples here.

**Theorem A.4.** *Let  $S$  be a densely defined, closed, symmetric operator in  $\mathfrak{H}$  decomposed in the form (A.7) and let  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  be a quasi boundary triple for  $\bar{T} = S^*$  with  $A_0 = T \upharpoonright \ker \Gamma_0$  and  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Assume that the extension  $A_1 = T \upharpoonright \ker \Gamma_1$  is self-adjoint in  $\mathfrak{H}$  and let  $B_0$  and  $B_1$  be self-adjoint operators as in (A.8). Furthermore, suppose that*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H}) \quad \text{for some } \lambda_0 \in \rho(A_0),$$

and that  $M(\lambda_1)^{-1}$  is a bounded operator in  $\mathcal{G}$  for some  $\lambda_1 \in \rho(A_0) \cap \rho(A_1)$ . Then (A.6) is satisfied for all  $\lambda \in \rho(A_0) \cap \rho(A_1)$  and the following assertions hold.

(i)  $\overline{\text{Im } M(\lambda)} \in \mathfrak{S}_1(\mathcal{G})$  for all  $\lambda \in \rho(A_0)$  and the limit

$$\overline{\text{Im } M(\lambda + i0)} := \lim_{\varepsilon \searrow 0} \overline{\text{Im } M(\lambda + i\varepsilon)}$$

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

(ii) For all  $\varphi \in \text{ran } \Gamma_0$  and a.e.  $\lambda \in \mathbb{R}$  the limit

$$M(\lambda \pm i0)\varphi := \lim_{\varepsilon \searrow 0} M(\lambda \pm i\varepsilon)\varphi$$

exists and the operators  $M(\lambda \pm i0)$  are closable with boundedly invertible closures  $\overline{M(\lambda \pm i0)}$ .

(iii) The space  $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$ , where

$$\mathcal{G}_\lambda := \text{ran} \left( \overline{\text{Im } M(\lambda + i0)} \right) \quad \text{for a.e. } \lambda \in \mathbb{R},$$

forms a spectral representation of  $A_0^{\text{ac}}$ .

(iv) The scattering matrix  $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$  of the scattering system  $\{A_0, A_1\}$  acting in the space  $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$  admits the representation

$$S(\lambda) = \begin{pmatrix} S'(\lambda) & 0 \\ 0 & I_{\mathcal{H}_\lambda} \end{pmatrix}$$

for a.e.  $\lambda \in \mathbb{R}$ , where

$$S'(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\overline{\text{Im } M(\lambda + i0)}} \left( \overline{M(\lambda + i0)} \right)^{-1} \sqrt{\overline{\text{Im } M(\lambda + i0)}}$$

is the scattering matrix of the scattering system  $\{B_0, B_1\}$ .

In the following, we show how the objects of this manuscript fit in the abstract scheme of quasi boundary triples. Let  $-\Delta_{\text{free}}$  be the self-adjoint Laplacian in  $L^2(\mathbb{R}^3)$  with domain  $H^2(\mathbb{R}^3)$  and let  $-\Delta_{\Sigma, \alpha}$  be the Schrödinger operator with a  $\delta$ -interaction of strength  $\frac{1}{\alpha}$  supported on  $\Sigma$  from Definition 2.3. Consider the symmetric operator

$$Su = -\Delta u, \quad \text{dom } S = \{u \in H^2(\mathbb{R}^3) : u|_\Sigma = 0\}, \quad (\text{A.9})$$

and define the operator  $T$  in  $L^2(\mathbb{R}^3)$  by

$$Tu = -\Delta u - h\delta_\Sigma, \quad \text{dom } T = H^2(\mathbb{R}^3) \dot{+} \{\gamma_\eta h : h \in \text{dom } \overline{B_\eta}\}, \quad (\text{A.10})$$

where  $\eta < 0$  is chosen such that  $0 \in \rho(\overline{B_\eta} - \alpha)$  (see Proposition 4.5 (ii) and (iv)) and  $\gamma_\eta h = (-\Delta - \eta)^{-1}(h\delta_\Sigma)$  is as in (2.3). It follows from the remark below Definition 2.2 that the sum in the definition of  $\text{dom } T$  is direct. Furthermore,  $T$

is a well-defined operator in  $L^2(\mathbb{R}^3)$  since for an element  $u = u_c + \gamma_\eta h \in \text{dom } T$  with  $u_c \in H^2(\mathbb{R}^3)$  and  $h \in \text{dom } \overline{B}_\eta$  one has

$$\begin{aligned}
 -\Delta u - h\delta_\Sigma &= (-\Delta - \eta)(u_c + \gamma_\eta h) + \eta(u_c + \gamma_\eta h) - h\delta_\Sigma \\
 &= -\Delta u_c + \eta\gamma_\eta h \in L^2(\mathbb{R}^3).
 \end{aligned}
 \tag{A.11}$$

Note also that

$$\ker(T - \eta) = \{\gamma_\eta h : h \in \text{dom } \overline{B}_\eta\}.
 \tag{A.12}$$

In the following useful proposition, we specify a quasi boundary triple  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  for the adjoint of the symmetric operator  $S$  such that  $-\Delta_{\text{free}} = T \upharpoonright \ker \Gamma_0$ .

**Proposition A.5.** *The operator  $S$  in (A.9) is densely defined, closed and symmetric in  $L^2(\mathbb{R}^3)$  and satisfies  $S^* = \overline{T}$  with  $T$  in (A.10). Furthermore, the triple  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$ , where*

$$\Gamma_0 u = h \quad \text{and} \quad \Gamma_1 u = u_c|_\Sigma, \quad u = u_c + \gamma_\eta h \in \text{dom } T,
 \tag{A.13}$$

is a quasi boundary triple for  $S^*$  such that  $\text{ran } \Gamma_0 = \text{dom } \overline{B}_\eta$ ,

$$-\Delta_{\text{free}} = T \upharpoonright \ker \Gamma_0 \quad \text{and} \quad -\Delta_{\Sigma, \alpha} = T \upharpoonright \ker (\Gamma_1 - (\alpha - \overline{B}_\eta)\Gamma_0).
 \tag{A.14}$$

The  $\gamma$ -field and Weyl function corresponding to  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  are given by

$$\gamma(\lambda)h = (-\Delta - \lambda)^{-1}(h\delta_\Sigma)
 \tag{A.15}$$

and

$$M(\lambda)h = [((-\Delta - \lambda)^{-1} - (-\Delta - \eta)^{-1})h\delta_\Sigma] \upharpoonright_\Sigma
 \tag{A.16}$$

for all  $\lambda \in \mathbb{C} \setminus [0, \infty)$  and  $h \in \text{dom } \overline{B}_\eta$ . The values  $M(\lambda)$  of the Weyl function are densely defined bounded operators in  $L^2(\Sigma)$ .

*Proof.* To show that the mappings in (A.13) yield a quasi boundary triple for  $S^*$ , we make use of Theorem A.2. Note first that the identities

$$S = T \upharpoonright (\ker \Gamma_0 \cap \ker \Gamma_1) \quad \text{and} \quad -\Delta_{\text{free}} = T \upharpoonright \ker \Gamma_0$$

hold. Hence, it remains to check that the Green identity

$$\langle Tu, v \rangle_{L^2(\mathbb{R}^3)} - \langle u, Tv \rangle_{L^2(\mathbb{R}^3)} = \langle \Gamma_1 u, \Gamma_0 v \rangle_{L^2(\Sigma)} - \langle \Gamma_0 u, \Gamma_1 v \rangle_{L^2(\Sigma)}
 \tag{A.17}$$

holds for all  $u, v \in \text{dom } T$  and that the range of the mapping  $u \mapsto (\Gamma_0 u, \Gamma_1 u)^\top$  is dense in  $L^2(\Sigma) \times L^2(\Sigma)$ . To verify (A.17) decompose  $u, v \in \text{dom } T$  in the form  $u = u_c + \gamma_\eta h$  and  $v = v_c + \gamma_\eta k$ , where  $u_c, v_c \in H^2(\mathbb{R}^3)$  and  $h, k \in \text{dom } \overline{B}_\eta$ .

With the help of (A.11), one computes

$$\begin{aligned}
 & \langle Tu, v \rangle_{L^2(\mathbb{R}^3)} - \langle u, Tv \rangle_{L^2(\mathbb{R}^3)} \\
 &= \langle T(u_c + \gamma_\eta h), v_c + \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} - \langle u_c + \gamma_\eta h, T(v_c + \gamma_\eta k) \rangle_{L^2(\mathbb{R}^3)} \\
 &= \langle -\Delta u_c + \eta \gamma_\eta h, v_c + \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} - \langle u_c + \gamma_\eta h, -\Delta v_c + \eta \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} \\
 &= \langle -\Delta u_c, \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} + \langle \eta \gamma_\eta h, v_c \rangle_{L^2(\mathbb{R}^3)} \\
 &\quad - \langle u_c, \eta \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} - \langle \gamma_\eta h, -\Delta v_c \rangle_{L^2(\mathbb{R}^3)} \\
 &= \langle (-\Delta - \eta)u_c, \gamma_\eta k \rangle_{L^2(\mathbb{R}^3)} - \langle \gamma_\eta h, (-\Delta - \eta)v_c \rangle_{L^2(\mathbb{R}^3)} \\
 &= \langle u_c, k \delta_\Sigma \rangle_{2,-2} - \langle h \delta_\Sigma, v_c \rangle_{-2,2} \\
 &= \langle u_c|_\Sigma, k \rangle_{L^2(\Sigma)} - \langle h, v_c|_\Sigma \rangle_{L^2(\Sigma)},
 \end{aligned}$$

which shows (A.17). Next assume that for some  $\varphi, \psi \in L^2(\Sigma)$

$$0 = \langle \varphi, \Gamma_0 u \rangle_{L^2(\Sigma)} + \langle \psi, \Gamma_1 u \rangle_{L^2(\Sigma)} = \langle \varphi, h \rangle_{L^2(\Sigma)} + \langle \psi, u_c|_\Sigma \rangle_{L^2(\Sigma)}$$

holds for all  $u = u_c + \gamma_\eta h \in \text{dom } T$ . Restricting to elements  $u$  in  $H^2(\mathbb{R}^3)$  (i.e.,  $h = 0$ ) it follows that  $\psi = 0$ . Finally, if  $0 = \langle \varphi, h \rangle_{L^2(\Sigma)}$  for all  $h \in \text{dom } \overline{B_\eta}$  then  $\varphi = 0$  as  $\overline{B_\eta}$  is densely defined in  $L^2(\Sigma)$ . Now it follows from Theorem A.2 that  $\overline{T} = S^*$  and that  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  is a quasi boundary triple for  $S^*$ .

To see that  $-\Delta_{\Sigma, \alpha} = T \upharpoonright \ker(\Gamma_1 - (\alpha - \overline{B_\eta})\Gamma_0)$  holds, suppose first that  $\Gamma_1 u = (\alpha - \overline{B_\eta})\Gamma_0 u$  or, equivalently,  $u_c|_\Sigma = (\alpha - \overline{B_\eta})h$  for some  $u = u_c + \gamma_\eta h \in \text{dom } T$ . Then it follows from the definition of  $u|_\Sigma$  in (2.8) that

$$u|_\Sigma = u_c|_\Sigma + (\gamma_\eta h)|_\Sigma = u_c|_\Sigma + \overline{B_\eta}h = \alpha h$$

and hence  $h = \frac{1}{\alpha}u|_\Sigma$ . Together with (A.10) and Definition 2.3 this implies

$$\ker(\Gamma_1 - (\alpha - \overline{B_\eta})\Gamma_0) \subset \text{dom}(-\Delta_{\Sigma, \alpha})$$

and  $-\Delta_{\Sigma, \alpha} u = Tu$  for all  $u \in \ker(\Gamma_1 - (\alpha - \overline{B_\eta})\Gamma_0)$ . If, conversely,  $u \in \text{dom}(-\Delta_{\Sigma, \alpha})$  then  $u = u_c + \gamma_\eta h$  for some  $u_c \in H^2(\mathbb{R}^3)$  and some  $h \in \text{dom } \overline{B_\eta}$ , in particular,  $u \in \text{dom } T$ . Moreover,

$$Tu = -\Delta u - h \delta_\Sigma \in L^2(\mathbb{R}^3)$$

and

$$-\Delta_{\Sigma, \alpha} u = -\Delta u - \frac{1}{\alpha}u|_\Sigma \cdot \delta_\Sigma \in L^2(\mathbb{R}^3),$$

which implies  $(h - \frac{1}{\alpha}u|_\Sigma)\delta_\Sigma \in L^2(\mathbb{R}^3)$  and thus  $h - \frac{1}{\alpha}u|_\Sigma = 0$ . Using again the definition of  $u|_\Sigma$  in (2.8) we obtain

$$0 = u|_\Sigma - \alpha h = u_c|_\Sigma + (\gamma_\eta h)|_\Sigma - \alpha h = u_c|_\Sigma - (\alpha - \overline{B_\eta})h$$

and thus  $u \in \ker(\Gamma_1 - (\alpha - \overline{B_\eta})\Gamma_0)$ . The second identity in (A.14) follows.

Next it will be shown that the  $\gamma$ -field and Weyl function corresponding to  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  have the form in (A.15) and (A.16). Note first that (A.12) and the definition of  $\Gamma_0$  imply  $\gamma(\eta)h = \gamma_\eta h = (-\Delta - \eta)^{-1}(h \delta_\Sigma)$  for all  $h \in$

$\text{ran } \Gamma_0 = \text{dom } \overline{B_\eta}$ . Furthermore, for  $\lambda \in \mathbb{C} \setminus [0, \infty)$ , we conclude from (A.3) and (A.14) that

$$\gamma(\lambda)h = (-\Delta_{\text{free}} - \eta)(-\Delta_{\text{free}} - \lambda)^{-1}\gamma(\eta)h = (-\Delta - \lambda)^{-1}(h\delta_\Sigma)$$

holds. Moreover,

$$\gamma(\lambda)^*u = \Gamma_1(-\Delta_{\text{free}} - \bar{\lambda})^{-1}u = ((-\Delta_{\text{free}} - \bar{\lambda})^{-1}u)|_\Sigma \tag{A.18}$$

for all  $u \in L^2(\mathbb{R}^3)$  by (A.2); cf. (2.5). It follows from the definition of  $\Gamma_1$  that

$$M(\eta)h = \Gamma_1\gamma(\eta)h = \Gamma_1(-\Delta - \eta)^{-1}(h\delta_\Sigma) = 0$$

holds for all  $h \in \text{ran } \Gamma_0 = \text{dom } \overline{B_\eta}$ . From (A.4) and (A.18) we then conclude for  $\lambda \in \mathbb{C} \setminus [0, \infty)$  and  $h \in \text{ran } \Gamma_0 = \text{dom } \overline{B_\eta}$

$$\begin{aligned} M(\lambda)h &= (\lambda - \eta)\gamma(\eta)^*(-\Delta_{\text{free}} - \eta)(-\Delta_{\text{free}} - \lambda)^{-1}\gamma(\eta)h \\ &= [(\lambda - \eta)(-\Delta_{\text{free}} - \lambda)^{-1}(-\Delta - \eta)^{-1}h\delta_\Sigma]|_\Sigma \\ &= [((-\Delta - \lambda)^{-1} - (-\Delta - \eta)^{-1})h\delta_\Sigma]|_\Sigma; \end{aligned}$$

cf. (4.26). We have shown that (A.16) holds. Note also that  $M(\eta) = 0$  and (A.4) with  $\mu = \eta$  imply that the operators  $M(\lambda)$  are bounded. This completes the proof of Proposition A.5. □

*Remark A.6.* If the operator  $T$  in (A.10) is replaced by the operator

$$T'u = -\Delta u - h\delta_\Sigma, \quad \text{dom } T' = H^2(\mathbb{R}^3) \dot{+} \{\gamma_\eta h : h \in L^2(\Sigma)\},$$

then  $T \subset T'$  and the assertions in Proposition A.5 remain valid with  $T$  replaced by  $T'$  and  $\text{dom } \overline{B_\eta}$  replaced by  $L^2(\Sigma)$ , respectively. In particular, in this situation the boundary map  $\Gamma_0$  maps onto  $L^2(\Sigma)$  and hence the quasi boundary triple  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  in Proposition A.5 is a generalized boundary triple, and the values  $M(\lambda)$  of the Weyl function are bounded operators defined on  $L^2(\Sigma)$ . It follows from (4.26) and (4.28) that

$$(M(\lambda)h)(x) = \int_\Sigma h(y) \frac{e^{i\sqrt{\lambda}|x-y|} - e^{i\sqrt{\eta}|x-y|}}{4\pi|x-y|} d\sigma(y), \quad x \in \Sigma, \quad h \in L^2(\Sigma).$$

Note, however, that  $\Gamma_1$  is not surjective and  $\{L^2(\Sigma), \Gamma_0, \Gamma_1\}$  is not an ordinary boundary triple.

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