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# Trace formulae and singular values of resolvent power differences of self-adjoint elliptic operators

Jussi Behrndt, Matthias Langer and Vladimir Lotoreichik

## ABSTRACT

In this note self-adjoint realizations of second order elliptic differential expressions with non-local Robin boundary conditions on a domain  $\Omega \subset \mathbb{R}^n$  with smooth compact boundary are studied. A Schatten–von Neumann type estimate for the singular values of the difference of the  $m$ th powers of the resolvents of two Robin realizations is obtained, and for  $m > \frac{n}{2} - 1$  it is shown that the resolvent power difference is a trace class operator. The estimates are slightly stronger than the classical singular value estimates by M. Sh. Birman where one of the Robin realizations is replaced by the Dirichlet operator. In both cases trace formulae are proved, in which the trace of the resolvent power differences in  $L^2(\Omega)$  is written in terms of the trace of derivatives of Neumann-to-Dirichlet and Robin-to-Neumann maps on the boundary space  $L^2(\partial\Omega)$ .

## 1. Introduction

Let  $\Omega \subset \mathbb{R}^n$  be a bounded or unbounded domain with smooth compact boundary and let  $\mathcal{L}$  be a formally symmetric second order elliptic differential expression with variable coefficients defined on  $\Omega$ . As a simple example one may consider  $\mathcal{L} = -\Delta$  or  $\mathcal{L} = -\Delta + V$  with some real function  $V$ . Denote by  $A_{\text{D}}$  the self-adjoint Dirichlet operator associated with  $\mathcal{L}$  in  $L^2(\Omega)$  and let  $A_{[\beta]}$  be a self-adjoint realization of  $\mathcal{L}$  in  $L^2(\Omega)$  with Robin boundary conditions of the form  $\beta f|_{\partial\Omega} = \frac{\partial f}{\partial\nu}|_{\partial\Omega}$  for functions  $f \in \text{dom } A_{[\beta]}$ . Here  $\beta$  is a real-valued bounded function on  $\partial\Omega$ ; in the special case  $\beta = 0$  one obtains the Neumann operator  $A_{\text{N}}$  associated with  $\mathcal{L}$ .

Half a century ago it was observed by M. Sh. Birman in his fundamental paper [9] that the difference of the resolvents of  $A_{\text{D}}$  and  $A_{[\beta]}$  is a compact operator whose singular values  $s_k$  satisfy  $s_k = O(k^{-\frac{2}{n-1}})$ ,  $k \rightarrow \infty$ , that is,

$$(A_{[\beta]} - \lambda)^{-1} - (A_{\text{D}} - \lambda)^{-1} \in \mathfrak{S}_{\frac{n-1}{2}, \infty}, \quad \lambda \in \rho(A_{[\beta]}) \cap \rho(A_{\text{D}}), \quad (1.1)$$

where  $\mathfrak{S}_{p, \infty}$  denotes the weak Schatten–von Neumann ideal of order  $p$ ; for the latter see (2.1) below. The difference of higher powers of the resolvents of  $A_{\text{D}}$  and  $A_{[\beta]}$  lead to stronger decay conditions of the form

$$(A_{[\beta]} - \lambda)^{-m} - (A_{\text{D}} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m}, \infty}, \quad \lambda \in \rho(A_{[\beta]}) \cap \rho(A_{\text{D}}); \quad (1.2)$$

see, e.g. [9, 25, 26, 27, 32]. The estimate (1.1) for the decay of the singular values is known to be sharp if  $\beta$  is smooth, see [10, 25, 26, 27], and [28] for the case  $\beta \in L^\infty(\partial\Omega)$ ; the estimate (1.2) is sharp for smooth  $\beta$  by [26, 27]. Observe that, for  $m > \frac{n-1}{2}$ , the operator in (1.2) belongs to the trace class ideal, and hence the wave operators for the scattering pair  $\{A_{\text{D}}, A_{[\beta]}\}$  exist and are complete, and the absolutely continuous parts of  $A_{\text{D}}$  and  $A_{[\beta]}$  are unitarily equivalent. A simple consequence of one of our main results in the present paper is

the following representation for the trace of the operator in (1.2) (see Theorem 3.10):

$$\begin{aligned} & \operatorname{tr}((A_{[\beta]} - \lambda)^{-m} - (A_{\text{D}} - \lambda)^{-m}) \\ &= \frac{1}{(m-1)!} \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( (I - M(\lambda)\beta)^{-1} M(\lambda)^{-1} M'(\lambda) \right) \right), \end{aligned} \quad (1.3)$$

where  $M(\lambda)$  is the Neumann-to-Dirichlet map (i.e. the inverse of the Dirichlet-to-Neumann map) associated with  $\mathcal{L}$ ; see also [7, Corollary 4.12] for  $m = 1$ . In the special case that  $A_{[\beta]}$  is the Neumann operator  $A_{\text{N}}$ , that is  $\beta = 0$ , the above formula simplifies to

$$\operatorname{tr}((A_{\text{N}} - \lambda)^{-m} - (A_{\text{D}} - \lambda)^{-m}) = \frac{1}{(m-1)!} \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( M(\lambda)^{-1} M'(\lambda) \right) \right), \quad (1.4)$$

which is an analogue of [14, Théorème 2.2] and reduces to [2, Corollary 3.7] in the case  $m = 1$ . We point out that the right-hand sides in (1.3) and (1.4) consist of traces of operators in the boundary space  $L^2(\partial\Omega)$ , whereas the left-hand sides are traces of operators in  $L^2(\Omega)$ . Some related reductions for ratios of Fredholm perturbation determinants can be found in [20]. We also refer to [17] for other types of trace formulae for Schrödinger operators.

Recently, it was shown in [6] that if one considers two self-adjoint Robin realizations  $A_{[\beta_1]}$  and  $A_{[\beta_2]}$  of  $\mathcal{L}$ , then the estimate (1.1) can be improved to

$$(A_{[\beta_1]} - \lambda)^{-1} - (A_{[\beta_2]} - \lambda)^{-1} \in \mathfrak{S}_{\frac{n-1}{3}, \infty}, \quad (1.5)$$

so that, roughly speaking, any two Robin realizations with bounded coefficients  $\beta_j$  are closer to each other than to the Dirichlet operator  $A_{\text{D}}$ ; see also [7] and the paper [28] by G. Grubb where the estimate (1.5) was shown to be sharp under some smoothness conditions on the functions  $\beta_1$  and  $\beta_2$ . One of the main objectives of this note is to prove a counterpart of (1.2) for higher powers of resolvents of  $A_{[\beta_1]}$  and  $A_{[\beta_2]}$ . For that we apply abstract boundary triple techniques from extension theory of symmetric operators and a variant of Krein’s formula which provides a convenient factorization of the resolvent difference of two self-adjoint realizations of  $\mathcal{L}$ ; cf. [4, 5, 7] and [12, 15, 18, 19, 24, 29, 32, 34, 35] for related approaches. Our tools allow us to consider general non-local Robin type realizations of  $\mathcal{L}$  of the form

$$\begin{aligned} & A_{[B]}f = \mathcal{L}f, \\ & \operatorname{dom} A_{[B]} = \left\{ f \in H^{3/2}(\Omega) : \mathcal{L}f \in L^2(\Omega), Bf|_{\partial\Omega} = \frac{\partial f}{\partial\nu} \Big|_{\partial\Omega} \right\}, \end{aligned} \quad (1.6)$$

where  $B$  is an arbitrary bounded self-adjoint operator in  $L^2(\partial\Omega)$  and  $H^{3/2}(\Omega)$  denotes the  $L^2$ -based Sobolev space of order  $3/2$ . In the special case where  $B$  is the multiplication operator with a bounded real-valued function  $\beta$  on  $\partial\Omega$  the differential operator in (1.6) coincides with the usual corresponding Robin realization  $A_{[\beta]}$  of  $\mathcal{L}$  in  $L^2(\Omega)$ . It is proved in Theorem 3.7 that for two self-adjoint realizations  $A_{[B_1]}$  and  $A_{[B_2]}$  as in (1.6) the difference of the  $m$ th powers of the resolvents satisfies

$$(A_{[B_1]} - \lambda)^{-m} - (A_{[B_2]} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1}, \infty}, \quad \lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}),$$

and if, in addition,  $B_1 - B_2$  belongs to some weak Schatten–von Neumann ideal, the estimate improves accordingly. Moreover, for  $m > \frac{n}{2} - 1$  the resolvent difference is a trace class operator and for the trace we obtain

$$\begin{aligned} & \operatorname{tr}((A_{[B_1]} - \lambda)^{-m} - (A_{[B_2]} - \lambda)^{-m}) \\ &= \frac{1}{(m-1)!} \operatorname{tr} \left[ \frac{d^{m-1}}{d\lambda^{m-1}} \left( (I - B_1 M(\lambda))^{-1} (B_1 - B_2) (I - M(\lambda) B_2)^{-1} M'(\lambda) \right) \right]. \end{aligned} \quad (1.7)$$

As in (1.3) and (1.4) the right-hand side in (1.7) consists of the trace of derivatives of Robin-to-Neumann and Neumann-to-Dirichlet maps on the boundary  $\partial\Omega$ , so that (1.7) can be viewed as a reduction of the trace in  $L^2(\Omega)$  to the boundary space  $L^2(\partial\Omega)$ .

The paper is organized as follows. We first recall some necessary facts about singular values and (weak) Schatten–von Neumann ideals in Section 2.1. In Section 2.2 the abstract concept of quasi boundary triples,  $\gamma$ -fields and Weyl functions from [4] is briefly recalled. Furthermore, we prove some preliminary results on the derivatives of the  $\gamma$ -field and Weyl function, and we provide some Krein-type formulae for the resolvent differences of self-adjoint extensions of a symmetric operator. Section 3 contains our main results on singular value estimates and traces of resolvent power differences of Dirichlet, Neumann and non-local Robin realizations of  $\mathcal{L}$ . In Section 3.1 the elliptic differential expression is defined and a family of self-adjoint Robin realizations is parameterized with the help of a quasi boundary triple. A detailed analysis of the smoothing properties of the derivatives of the corresponding  $\gamma$ -field and Weyl function together with Krein-type resolvent formulae and embeddings of Sobolev spaces then leads to the estimates and trace formulae in Theorems 3.6, 3.7 and 3.10.

## 2. Schatten–von Neumann ideals and quasi boundary triples

This section starts with preliminary facts on singular values and (weak) Schatten–von Neumann ideals. Furthermore, we review the concepts of quasi boundary triples, associated  $\gamma$ -fields and Weyl functions, which are convenient abstract tools for the parameterization and spectral analysis of self-adjoint realizations of elliptic differential expressions.

### 2.1. Singular values and Schatten–von Neumann ideals

Let  $\mathcal{H}$  and  $\mathcal{K}$  be Hilbert spaces. We denote by  $\mathcal{B}(\mathcal{H}, \mathcal{K})$  the space of bounded operators from  $\mathcal{H}$  to  $\mathcal{K}$  and by  $\mathfrak{S}_\infty(\mathcal{H}, \mathcal{K})$  the space of compact operators. Moreover, we set  $\mathcal{B}(\mathcal{H}) := \mathcal{B}(\mathcal{H}, \mathcal{H})$  and  $\mathfrak{S}_\infty(\mathcal{H}) := \mathfrak{S}_\infty(\mathcal{H}, \mathcal{H})$ .

The *singular values* (or *s-numbers*)  $s_k(K)$ ,  $k = 1, 2, \dots$ , of a compact operator  $K \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K})$  are defined as the eigenvalues of the non-negative compact operator  $(K^*K)^{1/2} \in \mathfrak{S}_\infty(\mathcal{H})$ , which are enumerated in non-increasing order and with multiplicities taken into account. Note that the singular values of  $K$  and  $K^*$  coincide:  $s_k(K) = s_k(K^*)$  for  $k = 1, 2, \dots$ ; see, e.g. [22, II.§2.2]. Recall that, for  $p > 0$ , the *Schatten–von Neumann ideals*  $\mathfrak{S}_p(\mathcal{H}, \mathcal{K})$  and *weak Schatten–von Neumann ideals*  $\mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K})$  are defined by

$$\begin{aligned} \mathfrak{S}_p(\mathcal{H}, \mathcal{K}) &:= \left\{ K \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K}) : \sum_{k=1}^{\infty} (s_k(K))^p < \infty \right\}, \\ \mathfrak{S}_{p,\infty}(\mathcal{H}, \mathcal{K}) &:= \left\{ K \in \mathfrak{S}_\infty(\mathcal{H}, \mathcal{K}) : s_k(K) = O(k^{-1/p}), k \rightarrow \infty \right\}. \end{aligned} \quad (2.1)$$

If no confusion can arise, the spaces  $\mathcal{H}$  and  $\mathcal{K}$  are suppressed and we write  $\mathfrak{S}_p$  and  $\mathfrak{S}_{p,\infty}$ . For  $0 < p' < p$  the inclusions

$$\mathfrak{S}_p \subset \mathfrak{S}_{p,\infty} \quad \text{and} \quad \mathfrak{S}_{p',\infty} \subset \mathfrak{S}_p \quad (2.2)$$

hold; for  $s, t > 0$  one has

$$\mathfrak{S}_{\frac{1}{s}} \cdot \mathfrak{S}_{\frac{1}{t}} = \mathfrak{S}_{\frac{1}{s+t}} \quad \text{and} \quad \mathfrak{S}_{\frac{1}{s},\infty} \cdot \mathfrak{S}_{\frac{1}{t},\infty} = \mathfrak{S}_{\frac{1}{s+t},\infty}, \quad (2.3)$$

where a product of operator ideals is defined as the set of all products. We refer the reader to [22, III.§7 and III.§14] and [36, Chapter 2] for a detailed study of the classes  $\mathfrak{S}_p$  and  $\mathfrak{S}_{p,\infty}$ ; see also [7, Lemma 2.3]. The ideal of *nuclear* or *trace class operators*  $\mathfrak{S}_1$  plays an important role later on. The trace of a compact operator  $K \in \mathfrak{S}_1(\mathcal{H})$  is defined as

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

where  $\lambda_k(K)$  are the eigenvalues of  $K$  and the sum converges absolutely. It is well known (see, e.g. [22, §III.8]) that, for  $K_1, K_2 \in \mathfrak{S}_1(\mathcal{H})$ ,

$$\operatorname{tr}(K_1 + K_2) = \operatorname{tr} K_1 + \operatorname{tr} K_2 \tag{2.4}$$

holds. Moreover, if  $K_1 \in \mathcal{B}(\mathcal{H}, \mathcal{K})$  and  $K_2 \in \mathcal{B}(\mathcal{K}, \mathcal{H})$  are such that  $K_1 K_2 \in \mathfrak{S}_1(\mathcal{K})$  and  $K_2 K_1 \in \mathfrak{S}_1(\mathcal{H})$ , then

$$\operatorname{tr}(K_1 K_2) = \operatorname{tr}(K_2 K_1). \tag{2.5}$$

The next useful lemma can be found in, e.g. [6, 7] and is based on the asymptotics of the eigenvalues of the Laplace–Beltrami operator. For a smooth compact manifold  $\Sigma$  we denote the usual  $L^2$ -based Sobolev spaces by  $H^r(\Sigma)$ ,  $r \geq 0$ .

**LEMMA 2.1.** *Let  $\Sigma$  be an  $(n - 1)$ -dimensional compact  $C^\infty$ -manifold without boundary, let  $\mathcal{K}$  be a Hilbert space and  $K \in \mathcal{B}(\mathcal{K}, H^{r_1}(\Sigma))$  with  $\operatorname{ran} K \subset H^{r_2}(\Sigma)$  where  $r_2 > r_1 \geq 0$ . Then  $K$  is compact and its singular values  $s_k(K)$  satisfy*

$$s_k(K) = O(k^{-\frac{r_2 - r_1}{n - 1}}), \quad k \rightarrow \infty,$$

*i.e.  $K \in \mathfrak{S}_{\frac{n-1}{r_2-r_1}, \infty}(\mathcal{K}, H^{r_1}(\Sigma))$  and hence  $K \in \mathfrak{S}_p(\mathcal{K}, H^{r_1}(\Sigma))$  for every  $p > \frac{n-1}{r_2-r_1}$ .*

## 2.2. Quasi boundary triples and their Weyl functions

In this subsection we recall the definitions and some important properties of quasi boundary triples, corresponding  $\gamma$ -fields and associated Weyl functions, cf. [4, 5, 7] for more details. Quasi boundary triples are particularly useful when dealing with elliptic boundary value problems from an operator and extension theoretic point of view.

**DEFINITION 2.2.** *Let  $A$  be a closed, densely defined, symmetric operator in a Hilbert space  $(\mathcal{H}, (\cdot, \cdot)_{\mathcal{H}})$ . A triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is called a quasi boundary triple for  $A^*$  if  $(\mathcal{G}, (\cdot, \cdot)_{\mathcal{G}})$  is a Hilbert space and for some linear operator  $T \subset A^*$  with  $\overline{T} = A^*$  the following holds:*

- (i)  $\Gamma_0, \Gamma_1 : \operatorname{dom} T \rightarrow \mathcal{G}$  are linear mappings, and the mapping  $\Gamma := \begin{pmatrix} \Gamma_0 \\ \Gamma_1 \end{pmatrix}$  has dense range in  $\mathcal{G} \times \mathcal{G}$ ;
- (ii)  $A_0 := T \upharpoonright \ker \Gamma_0$  is a self-adjoint operator in  $\mathcal{H}$ ;
- (iii) for all  $f, g \in \operatorname{dom} T$  the abstract Green identity holds:

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

We remark that a quasi boundary triple for  $A^*$  exists if and only if the deficiency indices of  $A$  coincide. Moreover, in the case of finite deficiency indices a quasi boundary triple is automatically an ordinary boundary triple, cf. [4, Proposition 3.3]. For the notion of (ordinary) boundary triples and their properties we refer to [13, 15, 16, 23, 30]. If  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is a quasi boundary triple for  $A^*$ , then  $A$  coincides with  $T \upharpoonright \ker \Gamma$  and the operator  $A_1 := T \upharpoonright \ker \Gamma_1$  is symmetric in  $\mathcal{H}$ . We also mention that a quasi boundary triple with the additional property  $\operatorname{ran} \Gamma_0 = \mathcal{G}$  is a generalized boundary triple in the sense of [16]; see [4, Corollary 3.7 (ii)].

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

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

holds for all  $\lambda \in \rho(A_0)$ , so that  $\Gamma_0 \upharpoonright \ker(T - \lambda)$  is invertible for all  $\lambda \in \rho(A_0)$ . The (operator-valued) functions  $\gamma$  and  $M$  defined by

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

are called the  $\gamma$ -field and the Weyl function corresponding to the quasi boundary triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ . These definitions coincide with the definitions of the  $\gamma$ -field and the Weyl function in the case that  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  is an ordinary boundary triple, see [15]. Note that, for each  $\lambda \in \rho(A_0)$ , the operator  $\gamma(\lambda)$  maps  $\text{ran } \Gamma_0 \subset \mathcal{G}$  into  $\text{dom } T \subset \mathcal{H}$  and  $M(\lambda)$  maps  $\text{ran } \Gamma_0$  into  $\text{ran } \Gamma_1$ . Furthermore, as an immediate consequence of the definition of  $M(\lambda)$ , we obtain

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

In the next proposition we collect some properties of the  $\gamma$ -field and the Weyl function associated with the quasi boundary triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  for  $A^*$ ; most statements were proved in [4].

**PROPOSITION 2.3.** *For all  $\lambda, \mu \in \rho(A_0)$  the following assertions hold.*

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

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

- (ii) *The mapping  $M(\lambda)$  is a densely defined (and in general unbounded) operator in  $\mathcal{G}$  that satisfies  $M(\lambda) \subset M(\bar{\lambda})^*$  and*

$$M(\lambda)h - M(\bar{\mu})h = (\lambda - \bar{\mu})\gamma(\mu)^*\gamma(\lambda)h$$

*for all  $h \in \mathcal{G}_0$ . If  $\text{ran } \Gamma_0 = \mathcal{G}$ , then  $M(\lambda) \in \mathcal{B}(\mathcal{G})$  and  $M(\lambda) = M(\bar{\lambda})^*$ .*

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

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

*Proof.* Items (i), (ii) and the first part of (iii) follow from [4, Proposition 2.6 (i), (ii), (iii), (v) and Corollary 3.7 (ii)]. For the second part of (iii) note that  $\{\mathcal{G}, \Gamma_1, -\Gamma_0\}$  is also a quasi boundary triple if  $A_1$  is self-adjoint. It is easy to see that in this case the corresponding  $\gamma$ -field is  $\tilde{\gamma}(\lambda) = \gamma(\lambda)M(\lambda)^{-1}$ . Since  $\text{ran}(\gamma(\bar{\lambda})^*) \subset \text{ran } \Gamma_1$  by item (ii), the operator  $M(\lambda)^{-1}\gamma(\bar{\lambda})^*$  is defined on  $\mathcal{H}$ . Now the boundedness of  $\tilde{\gamma}(\lambda)$ , which follows from (i), and the relation  $M(\lambda) \subset M(\bar{\lambda})^*$  imply that  $M(\lambda)^{-1}\gamma(\bar{\lambda})^*$  is bounded.  $\square$

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

$$\frac{d^m}{d\lambda^m}(A(\lambda)B(\lambda)) = \sum_{\substack{p+q=m \\ p, q \geq 0}} \binom{m}{p} A^{(p)}(\lambda)B^{(q)}(\lambda), \quad (2.6)$$

$$\frac{d^m}{d\lambda^m}(A(\lambda)B(\lambda)C(\lambda)) = \sum_{\substack{p+q+r=m \\ p, q, r \geq 0}} \frac{m!}{p!q!r!} A^{(p)}(\lambda)B^{(q)}(\lambda)C^{(r)}(\lambda) \quad (2.7)$$

for  $\lambda \in U$ . If  $A(\lambda)^{-1}$  is invertible for every  $\lambda \in U$ , then relation (2.6) implies the following formula for the derivative of the inverse,

$$\frac{d}{d\lambda}(A(\lambda)^{-1}) = -A(\lambda)^{-1}A'(\lambda)A(\lambda)^{-1}. \quad (2.8)$$

In the next lemma we consider higher derivatives of the  $\gamma$ -field and the Weyl function associated with a quasi boundary triple  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ .

LEMMA 2.4. *For all  $\lambda \in \rho(A_0)$  and all  $k \in \mathbb{N}$  the following holds.*

- (i)  $\frac{d^k}{d\lambda^k}\gamma(\bar{\lambda})^* = k!\gamma(\bar{\lambda})^*(A_0 - \lambda)^{-k}$ ;
- (ii)  $\frac{d^k}{d\lambda^k}\overline{\gamma(\lambda)} = k!(A_0 - \lambda)^{-k}\overline{\gamma(\lambda)}$ ;
- (iii)  $\frac{d^k}{d\lambda^k}M(\lambda) = \frac{d^{k-1}}{d\lambda^{k-1}}(\gamma(\bar{\lambda})^*\overline{\gamma(\lambda)}) = k!\gamma(\bar{\lambda})^*(A_0 - \lambda)^{-(k-1)}\overline{\gamma(\lambda)}$ .

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

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

where we used Proposition 2.3 (i). If we assume that the statement is true for  $k \in \mathbb{N}$ , then

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

which proves the statement in (i) by induction.

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

(iii) It follows from Proposition 2.3 (ii) that, for  $f \in \text{dom } M(\lambda) = \text{ran } \Gamma_0$ ,

$$\frac{d}{d\lambda}M(\lambda)f = \lim_{\mu \rightarrow \lambda} \frac{1}{\mu - \lambda} (M(\mu) - M(\lambda))f = \lim_{\mu \rightarrow \lambda} \gamma(\bar{\lambda})^*\gamma(\mu)f = \gamma(\bar{\lambda})^*\gamma(\lambda)f.$$

By taking closures we obtain the claim for  $k = 1$ . For  $k \geq 2$  we use (2.6) to get

$$\begin{aligned} \overline{\frac{d^k}{d\lambda^k} M(\lambda)} &= \overline{\frac{d^{k-1}}{d\lambda^{k-1}} \left( \gamma(\bar{\lambda})^* \overline{\gamma(\lambda)} \right)} = \sum_{\substack{p+q=k-1 \\ p, q \geq 0}} \binom{k-1}{p} \left( \frac{d^p}{d\lambda^p} \gamma(\bar{\lambda})^* \right) \frac{d^q}{d\lambda^q} \overline{\gamma(\lambda)} \\ &= \sum_{\substack{p+q=k-1 \\ p, q \geq 0}} \binom{k-1}{p} p! \gamma(\bar{\lambda})^* (A_0 - \lambda)^{-p} q! (A_0 - \lambda)^{-q} \overline{\gamma(\lambda)} \\ &= \sum_{\substack{p+q=k-1 \\ p, q \geq 0}} (k-1)! \gamma(\bar{\lambda})^* (A_0 - \lambda)^{-(k-1)} \overline{\gamma(\lambda)} = k! \gamma(\bar{\lambda})^* (A_0 - \lambda)^{-(k-1)} \overline{\gamma(\lambda)}, \end{aligned}$$

which finishes the proof.  $\square$

The following theorem provides a Krein-type formula for the resolvent difference of  $A_0$  and  $A_1$  if  $A_1$  is self-adjoint. The theorem follows from [4, Corollary 3.11 (i)] with  $\Theta = 0$ .

**THEOREM 2.5.** *Let  $A$  be a closed, densely defined, symmetric operator in a Hilbert space  $\mathcal{H}$  and let  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  be a quasi boundary triple for  $A^*$  with  $A_0 = T \upharpoonright \ker \Gamma_0$ ,  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Assume that  $A_1 = T \upharpoonright \ker \Gamma_1$  is self-adjoint in  $\mathcal{H}$ . Then*

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

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

Note that the operator  $M(\lambda)^{-1} \gamma(\bar{\lambda})^*$  in Theorem 2.5 above is bounded by Proposition 2.3 (iii).

In the following we deal with extensions of  $A$ , which are restrictions of  $T$  corresponding to some abstract boundary condition. For a linear operator  $B$  in  $\mathcal{G}$  we define

$$A_{[B]} f := T f, \quad \text{dom } A_{[B]} := \{f \in \text{dom } T : B \Gamma_1 f = \Gamma_0 f\}. \quad (2.9)$$

In contrast to ordinary boundary triples, self-adjointness of the parameter  $B$  does not imply self-adjointness of the corresponding extension  $A_{[B]}$  in general. The next theorem provides a useful sufficient condition for this and a variant of Krein's formula, which will be used later; see [5, Corollary 6.18 and Theorem 6.19] or [7, Corollary 3.11, Theorem 3.13 and Remark 3.14].

**THEOREM 2.6.** *Let  $A$  be a closed, densely defined, symmetric operator in a Hilbert space  $\mathcal{H}$  and let  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  be a quasi boundary triple for  $A^*$  with  $A_0 = T \upharpoonright \ker \Gamma_0$ ,  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Assume that  $\text{ran } \Gamma_0 = \mathcal{G}$ ,  $A_1 = T \upharpoonright \ker \Gamma_1$  is self-adjoint in  $\mathcal{H}$  and that  $M(\lambda_0) \in \mathfrak{S}_\infty(\mathcal{G})$  for some  $\lambda_0 \in \rho(A_0)$ .*

*If  $B$  is a bounded self-adjoint operator in  $\mathcal{G}$ , then the corresponding extension  $A_{[B]}$  is self-adjoint in  $\mathcal{H}$  and*

$$\begin{aligned} (A_{[B]} - \lambda)^{-1} - (A_0 - \lambda)^{-1} &= \gamma(\lambda) (I - B M(\lambda))^{-1} B \gamma(\bar{\lambda})^* \\ &= \gamma(\lambda) B (I - M(\lambda) B)^{-1} \gamma(\bar{\lambda})^* \end{aligned}$$

holds for  $\lambda \in \rho(A_{[B]}) \cap \rho(A_0)$  with

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



### 3. Elliptic operators on domains with compact boundaries

In this section we study self-adjoint realizations of elliptic second-order differential expressions on a bounded or an exterior domain subject to Robin or more general non-local boundary conditions. With the help of quasi boundary triple techniques we express the resolvent power differences of different self-adjoint realizations in Krein-type formulae. Using a detailed analysis of the perturbation term together with smoothing properties of the derivatives of the  $\gamma$ -fields and Weyl function we then obtain singular value estimates and trace formulae.

#### 3.1. Self-adjoint elliptic operators with non-local Robin boundary conditions

Let  $\Omega \subset \mathbb{R}^n$ ,  $n \geq 2$ , be a bounded or unbounded domain with a compact  $C^\infty$ -boundary  $\partial\Omega$ . We denote by  $(\cdot, \cdot)$  and  $(\cdot, \cdot)_{\partial\Omega}$  the inner products in the Hilbert spaces  $L^2(\Omega)$  and  $L^2(\partial\Omega)$ , respectively. Throughout this section we consider a formally symmetric second-order elliptic differential expression

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

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

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

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

For a function  $f \in C^\infty(\overline{\Omega})$  we denote the trace by  $f|_{\partial\Omega}$  and the (oblique) Neumann trace by

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

with the normal vector field  $\vec{\nu} = (\nu_1, \nu_2, \dots, \nu_n)$  pointing outwards  $\Omega$ . By continuity, the trace and the Neumann trace can be extended to mappings from  $H^s(\Omega)$  to  $H^{s-\frac{1}{2}}(\partial\Omega)$  for  $s > \frac{1}{2}$  and  $H^{s-\frac{3}{2}}(\partial\Omega)$  for  $s > \frac{3}{2}$ , respectively.

Next we define a quasi boundary triple for the adjoint  $A^*$  of the minimal operator

$$Af = \mathcal{L}f, \quad \text{dom } A = \{f \in H^2(\Omega) : f|_{\partial\Omega} = \partial_{\mathcal{L}} f|_{\partial\Omega} = 0\}$$

associated with  $\mathcal{L}$  in  $L^2(\Omega)$ . Recall that  $A$  is a closed, densely defined, symmetric operator with equal infinite deficiency indices and that

$$A^*f = \mathcal{L}f, \quad \text{dom } A^* = \{f \in L^2(\Omega) : \mathcal{L}f \in L^2(\Omega)\}$$

is the maximal operator associated with  $\mathcal{L}$ ; see, e.g. [1, 3]. As the operator  $T$  appearing in the definition of a quasi boundary triple we choose

$$Tf = \mathcal{L}f, \quad \text{dom } T = H_{\mathcal{L}}^{3/2}(\Omega) := \{f \in H^{3/2}(\Omega) : \mathcal{L}f \in L^2(\Omega)\}$$

and we consider the boundary mappings

$$\begin{aligned} \Gamma_0 : \text{dom } T &\rightarrow L^2(\partial\Omega), & \Gamma_0 f &:= \partial_{\mathcal{L}} f|_{\partial\Omega}, \\ \Gamma_1 : \text{dom } T &\rightarrow L^2(\partial\Omega), & \Gamma_1 f &:= f|_{\partial\Omega}. \end{aligned}$$

Note that the trace and the Neumann trace can be extended to mappings from  $H_{\mathcal{L}}^{3/2}(\Omega)$  into  $L^2(\partial\Omega)$ . With this choice of  $T$  and  $\Gamma_0$  and  $\Gamma_1$  we have the following proposition.

PROPOSITION 3.1. *The triple  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  is a quasi boundary triple for  $A^*$  with the Neumann and Dirichlet operator as self-adjoint operators corresponding to the kernels of the boundary mappings,*

$$\begin{aligned} A_N &:= T \upharpoonright \ker \Gamma_0, & \text{dom } A_N &= \{f \in H^2(\Omega) : \partial_{\mathcal{L}} f|_{\partial\Omega} = 0\}, \\ A_D &:= T \upharpoonright \ker \Gamma_1, & \text{dom } A_D &= \{f \in H^2(\Omega) : f|_{\partial\Omega} = 0\}. \end{aligned} \quad (3.1)$$

The ranges of the boundary mappings are

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

and the  $\gamma$ -field and Weyl function associated with  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  are given by

$$\gamma(\lambda)\varphi = f_\lambda \quad \text{and} \quad M(\lambda)\varphi = f_\lambda|_{\partial\Omega}, \quad \lambda \in \rho(A_N),$$

for  $\varphi \in L^2(\partial\Omega)$  where  $f_\lambda \in H_{\mathcal{L}}^{3/2}(\Omega)$  is the unique solution of the boundary value problem  $\mathcal{L}u = \lambda u$ ,  $\partial_{\mathcal{L}} u|_{\partial\Omega} = \varphi$ .

We remark that the quasi boundary triple  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  in Proposition 3.1 is a generalized boundary triple in the sense of [16] since the boundary mapping  $\Gamma_0$  is surjective.

*Proof.* The proof of Proposition 3.1 proceeds in the same way as the proof of [7, Theorem 4.2], except that here  $T$  is defined on the larger space  $H_{\mathcal{L}}^{3/2}(\Omega)$ . Therefore we do not repeat the arguments here, but provide only the main references that are necessary to translate the proof of [7, Theorem 4.2] to the present situation. The self-adjointness of  $A_D$  and  $A_N$  is ensured by [3, Theorem 7.1 (a)] and [11, Theorem 5 (iii)]. The trace theorem from [31, Chapter 2, §7.3] and the corresponding Green identity (see, e.g. [7, proof of Theorem 4.2]) yield the asserted properties of the ranges of the boundary mappings  $\Gamma_0$  and  $\Gamma_1$  and the abstract Green identity in Definition 2.2. Hence [4, Theorem 2.3] implies that the triple  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  in Proposition 3.1 is a quasi boundary triple for  $A^*$ ; cf. [7, Theorem 3.2, Theorem 4.2 and Proposition 4.3] for further details.  $\square$

The space  $H_{\text{loc}}^s(\overline{\Omega})$ ,  $s \geq 0$ , consists of all measurable functions  $f$  such that for any bounded open subset  $\Omega' \subset \Omega$  the condition  $f \upharpoonright \Omega' \in H^s(\Omega')$  holds. Since  $\Omega$  is a bounded domain or an exterior domain and  $\partial\Omega$  is compact, any function in  $H_{\text{loc}}^s(\overline{\Omega})$  is  $H^s$ -smooth up to the boundary  $\partial\Omega$ . For  $f \in H_{\text{loc}}^s(\overline{\Omega}) \cap L^2(\Omega)$ ,  $s \geq 0$ , our assumptions on the coefficients in the differential expression  $\mathcal{L}$  imply that

$$\begin{aligned} (A_D - \lambda)^{-1}f &\in H_{\text{loc}}^{s+2}(\overline{\Omega}) \cap L^2(\Omega), & \lambda &\in \rho(A_D), \\ (A_N - \lambda)^{-1}f &\in H_{\text{loc}}^{s+2}(\overline{\Omega}) \cap L^2(\Omega), & \lambda &\in \rho(A_N). \end{aligned} \quad (3.2)$$

These smoothing properties can be easily deduced from [33, Theorem 4.18], where they are formulated and proved in the language of boundary value problems.

The operators  $\gamma(\lambda)$  and  $M(\lambda)$  are also called *Poisson operator* and *Neumann-to-Dirichlet map* for the differential expression  $\mathcal{L} - \lambda$ . From Proposition 2.3 various properties of these operators can be deduced. In the next lemma we collect smoothing properties of these operators, which follow, basically, from Proposition 2.3 and the trace theorem for Sobolev spaces on smooth domains and its generalizations given in [31, Chapter 2].

LEMMA 3.2. *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Then, for all  $s \geq 0$ , the following statements hold.*

- (i)  $\text{ran}(\gamma(\lambda) \upharpoonright H^s(\partial\Omega)) \subset H_{\text{loc}}^{s+\frac{3}{2}}(\overline{\Omega}) \cap L^2(\Omega)$  for all  $\lambda \in \rho(A_N)$ ;
- (ii)  $\text{ran}(\gamma(\overline{\lambda})^* \upharpoonright H_{\text{loc}}^s(\overline{\Omega}) \cap L^2(\Omega)) \subset H^{s+\frac{3}{2}}(\partial\Omega)$  for all  $\lambda \in \rho(A_N)$ ;

- (iii)  $\text{ran}(M(\lambda) \upharpoonright H^s(\partial\Omega)) \subset H^{s+1}(\partial\Omega)$  for all  $\lambda \in \rho(A_N)$ ;  
(iv)  $\text{ran}(M(\lambda) \upharpoonright H^s(\partial\Omega)) = H^{s+1}(\partial\Omega)$  for all  $\lambda \in \rho(A_D) \cap \rho(A_N)$ .

*Proof.* (i) It follows from the decomposition  $\text{dom } T = \text{dom } A_N \dot{+} \ker(T - \lambda)$ ,  $\lambda \in \rho(A_N)$ , and the properties of the Neumann trace [31, Chapter 2, §7.3] that the restriction of the mapping  $\Gamma_0$  to

$$\ker(T - \lambda) \cap H_{\text{loc}}^{s+\frac{3}{2}}(\overline{\Omega})$$

is a bijection onto  $H^s(\partial\Omega)$ ,  $s \geq 0$ . Hence, by the definition of the  $\gamma$ -field, we obtain

$$\text{ran}(\gamma(\lambda) \upharpoonright H^s(\partial\Omega)) = \ker(T - \lambda) \cap H_{\text{loc}}^{s+\frac{3}{2}}(\overline{\Omega}) \subset H_{\text{loc}}^{s+\frac{3}{2}}(\overline{\Omega}) \cap L^2(\Omega).$$

- (ii) According to Proposition 2.3 (i) and the definition of  $\Gamma_1$  we have

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

Employing (3.2) and the properties of the Dirichlet trace [31, Chapter 2, §7.3] we conclude that

$$\text{ran}(\gamma(\overline{\lambda})^* \upharpoonright H_{\text{loc}}^s(\overline{\Omega}) \cap L^2(\Omega)) \subset H^{s+\frac{3}{2}}(\partial\Omega)$$

holds for all  $s \geq 0$ .

Assertion (iii) follows from the definition of  $M(\lambda)$ , item (i), the fact that  $\Gamma_1$  is the Dirichlet trace operator and properties of the latter.

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

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

that is,  $H^{s+1}(\partial\Omega) \subset \text{ran}(M(\lambda) \upharpoonright H^s(\partial\Omega))$ , and (iii) implies the assertion.  $\square$

In the next proposition we list some weak Schatten–von Neumann ideal properties of the derivatives of the  $\gamma$ -field and Weyl function, which follow from Lemma 2.4, elliptic regularity and Lemma 2.1.

**PROPOSITION 3.3.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Then the following statements hold.*

- (i) For all  $\lambda \in \rho(A_N)$  and  $k \in \mathbb{N}_0$ ,

$$\begin{aligned} \frac{d^k}{d\lambda^k} \gamma(\lambda) &\in \mathfrak{S}_{\frac{n-1}{2k+3/2}, \infty}(L^2(\partial\Omega), L^2(\Omega)), \\ \frac{d^k}{d\lambda^k} \gamma(\overline{\lambda})^* &\in \mathfrak{S}_{\frac{n-1}{2k+3/2}, \infty}(L^2(\Omega), L^2(\partial\Omega)). \end{aligned} \tag{3.3}$$

- (ii) For all  $\lambda \in \rho(A_N)$  and  $k \in \mathbb{N}_0$ ,

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

*Proof.* (i) Let  $\lambda \in \rho(A_N)$  and  $k \in \mathbb{N}_0$ . It follows from (3.2) that  $\text{ran}((A_N - \lambda)^{-k}) \subset H_{\text{loc}}^{2k}(\overline{\Omega}) \cap L^2(\Omega)$  and hence from Lemma 3.2 (ii) that

$$\text{ran}(\gamma(\overline{\lambda})^*(A_N - \lambda)^{-k}) \subset H^{2k+3/2}(\partial\Omega).$$

Thus Lemma 2.1 with  $\mathcal{K} = L^2(\Omega)$ ,  $\Sigma = \partial\Omega$ ,  $r_1 = 0$  and  $r_2 = 2k + 3/2$  implies that

$$\gamma(\bar{\lambda})^*(A_N - \lambda)^{-k} \in \mathfrak{S}_{\frac{n-1}{2k+3/2}, \infty}(L^2(\Omega), L^2(\partial\Omega)). \quad (3.4)$$

By taking the adjoint in (3.4) and replacing  $\lambda$  by  $\bar{\lambda}$  we obtain

$$(A_N - \lambda)^{-k}\gamma(\lambda) \in \mathfrak{S}_{\frac{n-1}{2k+3/2}, \infty}(L^2(\partial\Omega), L^2(\Omega)). \quad (3.5)$$

Now from Lemma 2.4 (i) and (ii) and (3.4) and (3.5) we obtain (3.3).

(ii) For  $k = 0$  we observe that  $\text{ran } M(\lambda) \subset H^1(\partial\Omega)$  by Lemma 3.2 (iii). Therefore Lemma 2.1 with  $\mathcal{K} = L^2(\partial\Omega)$ ,  $\Sigma = \partial\Omega$ ,  $r_1 = 0$  and  $r_2 = 1$  implies that  $M(\lambda) \in \mathfrak{S}_{n-1, \infty}(L^2(\partial\Omega))$ . For  $k \geq 1$  we have

$$\frac{d^k}{d\lambda^k} M(\lambda) = k! \gamma(\bar{\lambda})^*(A_N - \lambda)^{-(k-1)} \gamma(\lambda)$$

from Lemma 2.4 (iii). Hence (3.4) and (3.5) imply that

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

where the last equality follows from (2.3).  $\square$

As a consequence of Theorem 2.5 we obtain a factorization for the resolvent difference of self-adjoint operators  $A_N$  and  $A_D$ .

**COROLLARY 3.4.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with  $\gamma$ -field  $\gamma$  and Weyl function  $M$ . Then*

$$(A_N - \lambda)^{-1} - (A_D - \lambda)^{-1} = \gamma(\lambda)M(\lambda)^{-1}\gamma(\bar{\lambda})^*$$

holds for  $\lambda \in \rho(A_D) \cap \rho(A_N)$ .

Next we define a family of realizations of  $\mathcal{L}$  in  $L^2(\Omega)$  with general Robin-type boundary conditions of the form

$$A_{[B]}f := \mathcal{L}f, \quad \text{dom } A_{[B]} := \{f \in H_{\mathcal{L}}^{3/2}(\Omega) : Bf|_{\partial\Omega} = \partial_{\mathcal{L}}f|_{\partial\Omega}\}, \quad (3.6)$$

where  $B$  is a bounded self-adjoint operator in  $L^2(\partial\Omega)$ . In terms of the quasi boundary triple in Proposition 3.1 the operator  $A_{[B]}$  coincides with the one in (2.9), which is also equal to the restriction

$$T \upharpoonright \ker(B\Gamma_1 - \Gamma_0).$$

The following corollary is a consequence of Theorem 2.6 since  $\text{ran } \Gamma_0 = L^2(\partial\Omega)$ ,  $A_D$  is self-adjoint and  $M(\lambda)$  is compact for  $\lambda \in \rho(A_N)$  by Proposition 3.3 (ii).

**COROLLARY 3.5.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with  $\gamma$ -field  $\gamma$  and Weyl function  $M$ , and let  $B$  be a bounded self-adjoint operator in  $L^2(\partial\Omega)$ . Then the corresponding operator  $A_{[B]}$  in (3.6) is self-adjoint in  $L^2(\Omega)$  and*

$$(A_{[B]} - \lambda)^{-1} - (A_N - \lambda)^{-1} = \gamma(\lambda)(I - BM(\lambda))^{-1}B\gamma(\bar{\lambda})^* \quad (3.7)$$

$$= \gamma(\lambda)B(I - M(\lambda)B)^{-1}\gamma(\bar{\lambda})^* \quad (3.8)$$

holds for  $\lambda \in \rho(A_{[B]}) \cap \rho(A_N)$  with

$$(I - BM(\lambda))^{-1}, (I - M(\lambda)B)^{-1} \in \mathcal{B}(L^2(\partial\Omega)). \quad (3.9)$$

Note that the operators in (3.9) can be viewed as Robin-to-Neumann maps.

### 3.2. Operator ideal properties and traces of resolvent power differences

In this subsection we prove the main results of this note: estimates for the singular values of resolvent power differences of two self-adjoint realizations of the differential expression  $\mathcal{L}$  subject to Dirichlet, Neumann and non-local Robin boundary conditions.

The first theorem on the difference of the resolvent powers of the Dirichlet and Neumann operator is partially known from [9] and [26, 32], where the proof is based on variational principles, pseudo-differential methods or a reduction to higher order operators. Here we give an elementary, direct proof using our approach. In the case of first powers of the resolvents, the trace formula in item (ii) is contained in [2, 7]. An equivalent formula can also be found in [14], where it is used for the analysis of the Laplace–Beltrami operator on coupled manifolds.

**THEOREM 3.6.** *Let  $A_D$  and  $A_N$  be the self-adjoint Dirichlet and Neumann realization of  $\mathcal{L}$  in (3.1) and let  $M$  be the Weyl function from Proposition 3.1. Then the following statements hold.*

(i) *For all  $m \in \mathbb{N}$  and  $\lambda \in \rho(A_N) \cap \rho(A_D)$ ,*

$$(A_N - \lambda)^{-m} - (A_D - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m}, \infty}(L^2(\Omega)). \quad (3.10)$$

(ii) *If  $m > \frac{n-1}{2}$  then the resolvent power difference in (3.10) is a trace class operator and, for all  $\lambda \in \rho(A_N) \cap \rho(A_D)$ ,*

$$\mathrm{tr}\left((A_N - \lambda)^{-m} - (A_D - \lambda)^{-m}\right) = \frac{1}{(m-1)!} \mathrm{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\left(M(\lambda)^{-1}M'(\lambda)\right)\right).$$

*Proof.* (i) The proof of the first item is carried out in two steps.

*Step 1.* Let us introduce the operator function

$$S(\lambda) := M(\lambda)^{-1}\gamma(\bar{\lambda})^*, \quad \lambda \in \rho(A_N) \cap \rho(A_D).$$

Note that the product is well defined since  $\mathrm{ran}(\gamma(\bar{\lambda})^*) \subset H^1(\partial\Omega) = \mathrm{dom}(M(\lambda)^{-1})$ . Since  $A_D$  is self-adjoint, it follows from Proposition 2.3 (iii) that  $S(\lambda)$  is a bounded operator from  $L^2(\Omega)$  to  $L^2(\partial\Omega)$  for  $\lambda \in \rho(A_N) \cap \rho(A_D)$ . We prove the following smoothing property for the derivatives of  $S$ :

$$u \in H_{\mathrm{loc}}^s(\bar{\Omega}) \cap L^2(\Omega) \quad \Rightarrow \quad S^{(k)}(\lambda)u \in H^{s+2k+1/2}(\partial\Omega), \quad s \geq 0, k \in \mathbb{N}_0, \quad (3.11)$$

by induction. Since  $\gamma(\bar{\lambda})^*$  maps  $H_{\mathrm{loc}}^s(\bar{\Omega}) \cap L^2(\Omega)$  into  $H^{s+3/2}(\partial\Omega)$  for  $s \geq 0$  by Lemma 3.2 (ii) and  $M(\lambda)^{-1}$  maps  $H^{s+3/2}(\partial\Omega)$  into  $H^{s+1/2}(\partial\Omega)$  by Lemma 3.2 (iv), relation (3.11) is true for  $k = 0$ . Now let  $l \in \mathbb{N}_0$  and assume that (3.11) is true for every  $k = 0, 1, \dots, l$ . By (2.6), (2.8) and Lemma 2.4 (i), (iii) we have

$$\begin{aligned} S'(\lambda)u &= \frac{d}{d\lambda}(M(\lambda)^{-1})\gamma(\bar{\lambda})^*u + M(\lambda)^{-1}\frac{d}{d\lambda}\gamma(\bar{\lambda})^*u \\ &= -M(\lambda)^{-1}M'(\lambda)M(\lambda)^{-1}\gamma(\bar{\lambda})^*u + M(\lambda)^{-1}\gamma(\bar{\lambda})^*(A_N - \lambda)^{-1}u \\ &= -M(\lambda)^{-1}\gamma(\bar{\lambda})^*\gamma(\lambda)M(\lambda)^{-1}\gamma(\bar{\lambda})^*u + S(\lambda)(A_N - \lambda)^{-1}u \\ &= S(\lambda)(A_N - \lambda)^{-1}u - S(\lambda)\gamma(\lambda)S(\lambda)u \end{aligned}$$

for all  $u \in L^2(\Omega)$ . Hence, with the help of (2.6), (2.7) and Lemma 2.4 (ii), we obtain

$$\begin{aligned}
S^{(l+1)}(\lambda) &= \frac{d^l}{d\lambda^l} \left( S(\lambda)(A_N - \lambda)^{-1} - S(\lambda)\gamma(\lambda)S(\lambda) \right) \\
&= \sum_{\substack{p+q=l \\ p,q \geq 0}} \binom{l}{p} S^{(p)}(\lambda) \frac{d^q}{d\lambda^q} (A_N - \lambda)^{-1} - \sum_{\substack{p+q+r=l \\ p,q,r \geq 0}} \frac{l!}{p!q!r!} S^{(p)}(\lambda)\gamma^{(q)}(\lambda)S^{(r)}(\lambda) \\
&= \sum_{\substack{p+q=l \\ p,q \geq 0}} \frac{l!}{p!} S^{(p)}(\lambda)(A_N - \lambda)^{-(q+1)} - \sum_{\substack{p+q+r=l \\ p,q,r \geq 0}} \frac{l!}{p!r!} S^{(p)}(\lambda)(A_N - \lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda). \quad (3.12)
\end{aligned}$$

By the induction hypothesis, the smoothing property (3.2) and Lemma 3.2 (i), we have, for  $s \geq 0$  and  $p, q \geq 0, p + q = l$ ,

$$\begin{aligned}
u &\in H_{\text{loc}}^s(\bar{\Omega}) \cap L^2(\Omega) \\
&\implies (A_N - \lambda)^{-(q+1)}u \in H_{\text{loc}}^{s+2q+2}(\bar{\Omega}) \cap L^2(\Omega) \\
&\implies S^{(p)}(\lambda)(A_N - \lambda)^{-(q+1)}u \in H^{s+2q+2+2p+1/2}(\partial\Omega) = H^{s+2(l+1)+1/2}(\partial\Omega)
\end{aligned}$$

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

$$\begin{aligned}
u &\in H_{\text{loc}}^s(\bar{\Omega}) \cap L^2(\Omega) \\
&\implies S^{(r)}(\lambda)u \in H^{s+2r+1/2}(\partial\Omega) \\
&\implies \gamma(\lambda)S^{(r)}(\lambda)u \in H_{\text{loc}}^{s+2r+1/2+3/2}(\bar{\Omega}) \cap L^2(\Omega) \\
&\implies (A_N - \lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda)u \in H_{\text{loc}}^{s+2r+2+2q}(\bar{\Omega}) \cap L^2(\Omega) \\
&\implies S^{(p)}(\lambda)(A_N - \lambda)^{-q}\gamma(\lambda)S^{(r)}(\lambda)u \in H^{s+2r+2+2q+2p+1/2}(\partial\Omega) = H^{s+2(l+1)+1/2}(\partial\Omega),
\end{aligned}$$

which, together with (3.12), shows (3.11) for  $k = l + 1$  and hence, by induction, for all  $k \in \mathbb{N}_0$ . Therefore, an application of Lemma 2.1 yields that

$$S^{(k)}(\lambda) \in \mathfrak{S}_{\frac{n-1}{2k+1/2}, \infty}(L^2(\Omega), L^2(\partial\Omega)), \quad k \in \mathbb{N}_0, \lambda \in \rho(A_N) \cap \rho(A_D). \quad (3.13)$$

*Step 2.* Using Krein's formula from Corollary 3.4 and (2.6) we can write, for  $m \in \mathbb{N}$  and  $\lambda \in \rho(A_N) \cap \rho(A_D)$ ,

$$\begin{aligned}
(A_N - \lambda)^{-m} - (A_D - \lambda)^{-m} &= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} \left( (A_N - \lambda)^{-1} - (A_D - \lambda)^{-1} \right) \\
&= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} (\gamma(\lambda)S(\lambda)) \\
&= \frac{1}{(m-1)!} \sum_{\substack{p+q=m-1 \\ p,q \geq 0}} \binom{m-1}{p} \gamma^{(p)}(\lambda)S^{(q)}(\lambda). \quad (3.14)
\end{aligned}$$

Since, by Proposition 3.3 (i), (3.13) and (2.3),

$$\gamma^{(p)}(\lambda)S^{(q)}(\lambda) \in \mathfrak{S}_{\frac{n-1}{2p+3/2}, \infty} \cdot \mathfrak{S}_{\frac{n-1}{2q+1/2}, \infty} = \mathfrak{S}_{\frac{n-1}{2(p+q)+2}, \infty} = \mathfrak{S}_{\frac{n-1}{2m}, \infty} \quad (3.15)$$

for  $p, q$  with  $p + q = m - 1$ , we obtain (3.10).

(ii) If  $m > \frac{n-1}{2}$  then  $\frac{n-1}{2m} < 1$  and, by (2.2) and (3.15), each term in the sum in (3.14) is a trace class operator and, by a similar argument, also  $S^{(q)}(\lambda)\gamma^{(p)}(\lambda)$ . Hence the operator in (3.10) is a trace class operator, and we can apply the trace to (3.14) and use (2.4), (2.5) and

Lemma 2.4 (iii) to obtain

$$\begin{aligned}
(m-1)! \operatorname{tr} \left( (A_N - \lambda)^{-m} - (A_D - \lambda)^{-m} \right) &= \operatorname{tr} \left( \sum_{\substack{p+q=m-1 \\ p, q \geq 0}} \binom{m-1}{p} \gamma^{(p)}(\lambda) S^{(q)}(\lambda) \right) \\
&= \sum_{\substack{p+q=m-1 \\ p, q \geq 0}} \binom{m-1}{p} \operatorname{tr} \left( \gamma^{(p)}(\lambda) S^{(q)}(\lambda) \right) = \sum_{\substack{p+q=m-1 \\ p, q \geq 0}} \binom{m-1}{p} \operatorname{tr} \left( S^{(q)}(\lambda) \gamma^{(p)}(\lambda) \right) \\
&= \operatorname{tr} \left( \sum_{\substack{p+q=m-1 \\ p, q \geq 0}} \binom{m-1}{p} S^{(q)}(\lambda) \gamma^{(p)}(\lambda) \right) = \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( S(\lambda) \gamma(\lambda) \right) \right) \\
&= \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( M(\lambda)^{-1} \gamma(\bar{\lambda})^* \gamma(\lambda) \right) \right) = \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( M(\lambda)^{-1} M'(\lambda) \right) \right),
\end{aligned}$$

which finishes the proof.  $\square$

In the following theorem, which contains the main result of this note, we prove weak Schatten–von Neumann estimates for resolvent power differences of two self-adjoint realizations  $A_{[B_1]}$  and  $A_{[B_2]}$  of  $\mathcal{L}$  with Robin and more general non-local boundary conditions. In this situation the estimates are better than for the pair of Dirichlet and Neumann realizations in Theorem 3.6. For the first powers of the resolvents this was already observed in [6, 7] and [28]. In the special important case when the resolvent power difference is a trace class operator we express its trace as the trace of a certain operator acting on the boundary  $\partial\Omega$ , which is given in terms of the Weyl function and the operators  $B_1$  and  $B_2$  in the boundary conditions; cf. [7, Corollary 4.12] for the case of first powers and [8, 21] for one-dimensional Schrödinger operators and other finite-dimensional situations. We also mention that the special case of classical Robin boundary conditions, where  $B_1$  and  $B_2$  are multiplication operators with real-valued  $L^\infty$ -functions is contained in the theorem.

**THEOREM 3.7.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with Weyl function  $M$  and let  $A_N$  be the self-adjoint Neumann operator in (3.1). Moreover, let  $B_1$  and  $B_2$  be bounded self-adjoint operators in  $L^2(\partial\Omega)$ , define  $A_{[B_1]}$  and  $A_{[B_2]}$  as in (3.6) and set*

$$t := \begin{cases} \frac{n-1}{s} & \text{if } B_1 - B_2 \in \mathfrak{S}_{s, \infty}(L^2(\partial\Omega)) \text{ for some } s > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then the following statements hold.

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

$$(A_{[B_1]} - \lambda)^{-m} - (A_{[B_2]} - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+t+1}, \infty}(L^2(\Omega)). \quad (3.16)$$

(ii) If  $m > \frac{n-t}{2} - 1$  then the resolvent power difference in (3.16) is a trace class operator and, for all  $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \rho(A_N)$ ,

$$\operatorname{tr} \left( (A_{[B_1]} - \lambda)^{-m} - (A_{[B_2]} - \lambda)^{-m} \right) = \frac{1}{(m-1)!} \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( U(\lambda) M'(\lambda) \right) \right) \quad (3.17)$$

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

*Proof.* (i) In order to shorten notation and to avoid the distinction of several cases, we set

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

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

$$\mathfrak{A}_{r_1} \cdot \mathfrak{A}_{r_2} = \mathfrak{A}_{r_1+r_2}, \quad r_1, r_2 \geq 0. \quad (3.18)$$

Moreover, the assumption on the difference of  $B_1$  and  $B_2$  yields

$$B_1 - B_2 \in \mathfrak{A}_t. \quad (3.19)$$

The proof of item (i) is divided into three steps.

*Step 1.* Let  $B$  be a bounded self-adjoint operator in  $L^2(\partial\Omega)$  and set

$$T(\lambda) := (I - BM(\lambda))^{-1}, \quad \lambda \in \rho(A_{[B]}) \cap \rho(A_N),$$

where  $T(\lambda) \in \mathcal{B}(L^2(\partial\Omega))$  by Corollary 3.5. We show that

$$T^{(k)}(\lambda) \in \mathfrak{A}_{2k+1}, \quad k \in \mathbb{N}, \quad (3.20)$$

by induction. Relation (2.8) implies that

$$T'(\lambda) = T(\lambda)BM'(\lambda)T(\lambda), \quad (3.21)$$

which is in  $\mathfrak{A}_3$  by Proposition 3.3 (ii). Let  $l \in \mathbb{N}$  and assume that (3.20) is true for every  $k = 1, \dots, l$ , which implies in particular that

$$T^{(k)}(\lambda) \in \mathfrak{A}_{2k}, \quad k = 0, \dots, l. \quad (3.22)$$

Then

$$T^{(l+1)}(\lambda) = \frac{d^l}{d\lambda^l} \left( T(\lambda)BM'(\lambda)T(\lambda) \right) = \sum_{\substack{p+q+r=l \\ p, q, r \geq 0}} \frac{l!}{p!q!r!} T^{(p)}(\lambda)BM^{(q+1)}(\lambda)T^{(r)}(\lambda)$$

by (3.21) and (2.7). Relation (3.22), the boundedness of  $B$ , Proposition 3.3 (ii) and (3.18) imply that

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

since  $p + q + r = l$ . This shows (3.20) for  $k = l + 1$  and hence, by induction, for all  $k \in \mathbb{N}$ . Since  $T(\lambda) \in \mathcal{B}(L^2(\partial\Omega))$ , we have

$$T^{(k)}(\lambda) \in \mathfrak{A}_{2k}, \quad k \in \mathbb{N}_0, \quad \lambda \in \rho(A_N), \quad (3.23)$$

and by similar considerations also

$$\frac{d^k}{d\lambda^k} (I - M(\lambda)B)^{-1} \in \mathfrak{A}_{2k}, \quad k \in \mathbb{N}_0, \quad \lambda \in \rho(A_N). \quad (3.24)$$

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

$$T_1(\lambda) := (I - B_1M(\lambda))^{-1} \quad \text{and} \quad T_2(\lambda) := (I - M(\lambda)B_2)^{-1}$$

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

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

By (3.23), (3.24) and (3.19), each term in the sum satisfies

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



and hence

$$U^{(k)}(\lambda) \in \mathfrak{A}_{2k+t}, \quad k \in \mathbb{N}_0, \lambda \in \rho(A_N). \quad (3.25)$$

*Step 3.* By applying (3.7) to  $A_{[B_1]}$  and (3.8) to  $A_{[B_2]}$  and taking the difference we obtain that, for  $\lambda \in \rho(A_{[B_1]}) \cap \rho(A_{[B_2]}) \cap \rho(A_N)$ ,

$$\begin{aligned} & (A_{[B_1]} - \lambda)^{-1} - (A_{[B_2]} - \lambda)^{-1} \\ &= \gamma(\lambda) \left[ (I - B_1 M(\lambda))^{-1} B_1 - B_2 (I - M(\lambda) B_2)^{-1} \right] \gamma(\bar{\lambda})^* \\ &= \gamma(\lambda) \left[ (I - B_1 M(\lambda))^{-1} B_1 (I - M(\lambda) B_2) (I - M(\lambda) B_2)^{-1} \right. \\ &\quad \left. - (I - B_1 M(\lambda))^{-1} (I - B_1 M(\lambda)) B_2 (I - M(\lambda) B_2)^{-1} \right] \gamma(\bar{\lambda})^* \\ &= \gamma(\lambda) \left[ (I - B_1 M(\lambda))^{-1} (B_1 - B_2) (I - M(\lambda) B_2)^{-1} \right] \gamma(\bar{\lambda})^* = \gamma(\lambda) U(\lambda) \gamma(\bar{\lambda})^*. \end{aligned}$$

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

$$\begin{aligned} & (A_{[B_1]} - \lambda)^{-m} - (A_{[B_2]} - \lambda)^{-m} \\ &= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} \left( (A_{[B_1]} - \lambda)^{-1} - (A_{[B_2]} - \lambda)^{-1} \right) \\ &= \frac{1}{(m-1)!} \cdot \frac{d^{m-1}}{d\lambda^{m-1}} \left( \gamma(\lambda) U(\lambda) \gamma(\bar{\lambda})^* \right) \\ &= \frac{1}{(m-1)!} \sum_{\substack{p+q+r=m-1 \\ p, q, r \geq 0}} \frac{(m-1)!}{p! q! r!} \gamma^{(p)}(\lambda) U^{(q)}(\lambda) \frac{d^r}{d\lambda^r} \gamma(\bar{\lambda})^*. \end{aligned} \quad (3.26)$$

By Proposition 3.3 (i) and (3.25), each term in the sum satisfies

$$\gamma^{(p)}(\lambda) U^{(q)}(\lambda) \frac{d^r}{d\lambda^r} \gamma(\bar{\lambda})^* \in \mathfrak{S}_{\frac{n-1}{2p+3/2}, \infty} \cdot \mathfrak{S}_{\frac{n-1}{2q+t}, \infty} \cdot \mathfrak{S}_{\frac{n-1}{2r+3/2}, \infty} = \mathfrak{S}_{\frac{n-1}{2m+t+1}, \infty}, \quad (3.27)$$

which proves (3.16).

(ii) If  $m > \frac{n-t}{2} - 1$  then  $\frac{n-1}{2m+t+1} < 1$  and, by (2.2) and (3.27), all terms in the sum in (3.26) are trace class operators, and the same is true if we change the order in the product in (3.27). Hence we can apply the trace to the expression in (3.26) and use (2.4), (2.5) and Lemma 2.4 (iii) to obtain

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

$$\begin{aligned}
&= \operatorname{tr} \left( \sum_{\substack{p+q+r=m-1 \\ p,q,r \geq 0}} \frac{(m-1)!}{p!q!r!} U^{(q)}(\lambda) \left( \frac{d^r}{d\lambda^r} \gamma(\bar{\lambda})^* \right) \gamma^{(p)}(\lambda) \right) \\
&= \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( U(\lambda) \gamma(\bar{\lambda})^* \gamma(\lambda) \right) \right) = \operatorname{tr} \left( \frac{d^{m-1}}{d\lambda^{m-1}} \left( U(\lambda) M'(\lambda) \right) \right),
\end{aligned}$$

which shows (3.17).  $\square$

**REMARK 3.8.** *The statements of Theorem 3.7 remain true if  $A$  is an arbitrary closed symmetric operator in a Hilbert space  $\mathcal{H}$  and  $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$  a quasi boundary triple for  $A^*$  such that  $\operatorname{ran} \Gamma_0 = \mathcal{G}$  and the statements of Proposition 3.3 are true with  $L^2(\Omega)$  and  $L^2(\partial\Omega)$  replaced by  $\mathcal{H}$  and  $\mathcal{G}$ , respectively.*

As a special case of the last theorem let us consider the situation when  $B_1 = B$  and  $B_2 = 0$ , where  $B$  is a bounded self-adjoint operator in  $L^2(\partial\Omega)$ . This immediately leads to the following corollary.

**COROLLARY 3.9.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with Weyl function  $M$  and let  $A_N$  be the self-adjoint Neumann operator in (3.1). Moreover, let  $B$  be a bounded self-adjoint operator in  $L^2(\partial\Omega)$ , define  $A_{[B]}$  as in (3.6) and set*

$$t := \begin{cases} \frac{n-1}{s} & \text{if } B \in \mathfrak{S}_{s,\infty}(L^2(\partial\Omega)) \text{ for some } s > 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then the following statements hold.

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

$$(A_{[B]} - \lambda)^{-m} - (A_N - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+t+1}, \infty}(L^2(\Omega)),$$

(ii) If  $m > \frac{n-t}{2} - 1$  then the resolvent power difference in (3.28) is a trace class operator and, for all  $\lambda \in \rho(A_{[B]}) \cap \rho(A_N)$ ,

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

The following theorem, where we compare operators with non-local and Dirichlet boundary conditions, is a consequence of Theorems 3.6 and 3.7.

**THEOREM 3.10.** *Let  $\{L^2(\partial\Omega), \Gamma_0, \Gamma_1\}$  be the quasi boundary triple from Proposition 3.1 with Weyl function  $M$  and let  $A_D$  be the self-adjoint Dirichlet operator in (3.1). Moreover, let  $B$  be a bounded self-adjoint operator in  $L^2(\partial\Omega)$  and define  $A_{[B]}$  as in (3.6). Then the following statements hold.*

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

$$(A_{[B]} - \lambda)^{-m} - (A_D - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m}, \infty}(L^2(\Omega)). \quad (3.28)$$

- (ii) If  $m > \frac{n-1}{2}$  then the resolvent power difference in (3.28) is a trace class operator and, for all  $\lambda \in \rho(A_{[B]}) \cap \rho(A_D) \cap \rho(A_N)$ ,

$$\operatorname{tr}\left((A_{[B]} - \lambda)^{-m} - (A_D - \lambda)^{-m}\right) = \frac{1}{(m-1)!} \operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\left(V(\lambda)M'(\lambda)\right)\right) \quad (3.29)$$

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

*Proof.* (i) Let us fix  $\lambda \in \rho(A_{[B]}) \cap \rho(A_D) \cap \rho(A_N)$ . From Theorems 3.6 (i) and 3.7 (i) it follows that

$$X_1(\lambda) := (A_N - \lambda)^{-m} - (A_D - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m}, \infty},$$

$$X_2(\lambda) := (A_{[B]} - \lambda)^{-m} - (A_N - \lambda)^{-m} \in \mathfrak{S}_{\frac{n-1}{2m+1}, \infty} \subset \mathfrak{S}_{\frac{n-1}{2m}, \infty},$$

and thus

$$(A_{[B]} - \lambda)^{-m} - (A_D - \lambda)^{-m} = X_1(\lambda) + X_2(\lambda) \in \mathfrak{S}_{\frac{n-1}{2m}, \infty}.$$

By analyticity we can extend this to all points  $\lambda$  in  $\rho(A_{[B]}) \cap \rho(A_D)$ .

- (ii) If  $m > \frac{n-1}{2}$ , then  $\frac{n-1}{2m} < 1$  and hence, by item (i) and (2.2), the operator in (3.28) is a trace class operator. Using Theorem 3.6 (ii) and Corollary 3.9 (ii) we obtain

$$\begin{aligned} \operatorname{tr}\left((A_{[B]} - \lambda)^{-m} - (A_D - \lambda)^{-m}\right) &= \operatorname{tr}(X_1(\lambda) + X_2(\lambda)) \\ &= \frac{1}{(m-1)!} \operatorname{tr}\left(\frac{d^{m-1}}{d\lambda^{m-1}}\left[\left(M(\lambda)^{-1} + (I - BM(\lambda))^{-1}B\right)M'(\lambda)\right]\right). \end{aligned}$$

Since

$$\begin{aligned} &M(\lambda)^{-1} + (I - BM(\lambda))^{-1}B \\ &= (I - BM(\lambda))^{-1}\left[(I - BM(\lambda)) + BM(\lambda)\right]M(\lambda)^{-1} = V(\lambda), \end{aligned}$$

this implies (3.29).  $\square$

Note that, for  $B$  being a multiplication operator by a bounded function  $\beta$ , the statement in (i) of the previous theorem is exactly the estimate (1.2).

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